Maharaja's College Ernakulam

A GOVERNMENT AUTONOMOUS COLLEGE

Re-Accredited by NAAC with 'A Grade'
Affiliated to Mahatma Gandhi University
Centre of Excellence under Govt. of Kerala
Identified by UGC as College with Potential for Excellence

POST GRADUATE & RESEARCH DEPARTMENT OF CHEMISTRY

Post Graduate Curriculum and Syllabus

(All Branches)

For 2019 Admission Onwards

M.Sc. PHARMACEUTICAL CHEMISTRY

FOREWORD

The Board of Studies in Chemistry take this opportunity to express our deep appreciation to all academicians and professionals who participated in the series of workshops organized by the Board for restructuring curriculum and syllabi of the PG courses in Chemistry - M.Sc Chemistry, M.Sc Analytical Chemistry, M.Sc Pharmaceutical Chemistry and M.Sc Applied Chemistry. We express our profound gratitude to the Honourable Vice-Chancellor, Pro-Vice Chancellor, Members of the Syndicate and Members of the Academic Council, Mahatma Gandhi University, for their sincere co-operation and guidance for completion of this work. Our special thanks are due to Chairman and members of the Governing Council, Chairman and members of the Academic Council, Maharaja's College, Ernakulam.

We also extend our gratitude to Prof. (Dr). K. K. Mohammed Yusuff, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). S. Sugunan, Professor (Retd.), Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Girish Kumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Prof. (Dr). K. Sreekumar, Professor, Department of Applied Chemistry, Cochin University of Science and Technology, Dr. E. Prasad, Associate Professor, Department of Chemistry, IIT, Madras, Dr. Kochubaby Manjooran, Dy.Manager (Energy and Envt), BPCL, Kochi Refinery, Sri. M. G. Rajagopalan, Associate Professor (Retd.) Maharaja's College, Ernakulam, Smt. K. T. Geethabali, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. T. Narayanan, Associate Professor (Retd.), Maharaja's College, Ernakulam, Dr. Lissamma Koshy, Associate Professor (Retd.), Maharaja's College, Ernakulam and Dr. Anitha I, Principal, KKTM College, Pullut who were entrusted with the responsibility as experts for the revision of the syllabus of different subjects. The Board of Studies in Chemistry expresses the whole hearted gratitude to all those who have helped in this endeavour.

The task of preparing the curricula and syllabi and bringing it out in the present form for all the four M.Sc courses was not simple but it was possible with dedicated efforts and wholehearted support and involvement of all the members of the BOS and the faculty members of the Department of Chemistry. I would like to express my sincere thanks to all my fellow members of BOS and the faculty members of the Department of Chemistry for all their help, cooperation, encouragement, active participation and useful suggestions for the completion of syllabus.

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PROGRAMME STRUCTURE

Examination

- There shall be end semester examination at the end of each semester.
- The answers must be written in English except for those coming under Faculty of Languages.
- Practical examinations shall be conducted by the college at the end of even semesters only.
- Project evaluation and Viva -Voce shall be conducted at the end of the programme only.
- Practical examination, Project evaluation and Viva-Voce shall be conducted by two external examiners.

END-Semester Examination

- The examinations shall normally at the end of each semester. There shall be one end-semester examination of 3 hours duration in each lecture based course and practical course.
- A question paper may contain short answer type/annotation, short essay type questions/problems and long essay type questions.

Evaluation and Grading

Evaluation

The evaluation scheme for each course shall contain two parts; (a) in-semester evaluation and (b) end-semester evaluation. 20 marks shall be given to in-semester evaluation and the remaining 80 marks to end-semester evaluation. Both in-semester and end semester evaluation shall be carried out by using in mark system. Both internal and external marks are to be mathematically rounded to the nearest integer.

Internal evaluation

The internal evaluation shall be based on predetermined transparent system involving periodic written tests, assignments, seminars and attendance in respect of theory courses and based on written tests, lab skill/records/viva and attendance in respect of practical courses. The marks assigned to various components for in-semester evaluation is as follows.

Components of In-semester Evaluation (For theory)

Components	Component Marks
Assignment	4
Seminar	4
Two Test papers*	8
Attendance	4
Total	20

*Marks of Test Papers shall be the average

Components of In-semester Evaluation (For Practical)

Components	Component Marks
Attendance	4
Laboratory Involvement	4
Written/Lab Test	4
Record*	4
Viva	4
Total	20

*Marks awarded to Record should be related to number of experiments recorded

Components of In-semester Evaluation (For Project)

Components	Marks
Topic/Area selected	2
Experimentation/Data collection	4
Punctuality	2
Compilation	4
Content	4
Presentation	4
Total	**20**

a) Evaluation of Attendance

% of attendance	Mark
95 and above	4
85 to 94	3
80 to 84	2
75 to 79	1
< 75	0

(Decimals are to be rounded to the next higher whole number)

a) Evaluation of Assignment

Components	Marks
Punctuality	1
Content	1
Conclusion	1
Reference/Review	1
Total	**4**

b) Evaluation of Seminar

Components	Marks
Content	1
Presentation	2
Reference/Review	1
Total	**4**

To ensure transparency of the evaluation process, the in-semester marks awarded to the students in each course in a semester shall be published on the notice board at least one week before the commencement of external examination. There shall not be any chance for improvement for in semester marks. The course teacher and the faculty advisor shall maintain the academic record of each student registered for the course and a copy should be kept in the college for at least one year for verification.

End-Semester Evaluation:

The end-semester evaluation in theory courses is to be conducted by the college with question papers set by external experts. The answers must be written in English except those for the Faculty of Languages. The evaluation of the answer scripts shall be done by examiners based on a well-defined scheme of valuation. The end-semester evaluation shall be done immediately after the examination preferably through Centralized Valuation.

Photocopies of the answer scripts of the external examination shall be made available to the students for scrutiny on request and revaluation/scrutiny of answer scripts shall be done as per the request of the candidate by paying fees.

The question paper should be strictly on the basis of model question paper set by BOS and there shall be a combined meeting of the question paper setters for scrutiny and finalization of question paper. Each set of question should be accompanied by its answer scheme for valuation.

Pattern of Questions

The question setter shall ensure that questions to course should satisfy weightage to objectives and weightage to difficulty levels.

Weightage to Objectives	
Objectives	**%**
Understanding	25
Critical Evaluation	50
Application	25

Weightage to difficulty levels	
Level of difficulty	**%**
Easy	20
Average	60
Difficult	20

Question paper setters shall also submit a detailed scheme of evaluation along with the question paper. A question paper shall be a judicious mix of objective type, short answer type, short essay type /problem solving type and long essay type questions.

Pattern of questions for end semester examination

	Total no. of questions	**Number of questions to be answered**	**Marks of each question**	**Total marks**
	12	10	2	20
	10	6	5	30
	4	2	15	30
TOTAL	**26**	**18**	x	**80**

Grades for Courses

For all courses (theory & practical), grades are given on a 10-point scale based on the total percentage of marks ***(ISA+ESA)*** as given below

Percentage of Marks	Grade	Grade Point (GP)
95 and above	S Outstanding	10
85 to below 95	A^+ Excellent	9
75 to below 85	A Very Good	8
65 to below 75	A- Good	7
55 to below 65	B^+ Above Average	6
50 to below 55	B Average	5
40 to below 50	C Pass	4
Below 40	F Fail	0
	Ab Absent	0

Credit Point and Credit Point Average:

Credit Point (CP) of a course is calculated using the formula

CP = C × GP, where C = Credit; GP = Grade point

Semester Grade Point Average (SGPA) of a Semester is calculated using the formula

SGPA= TCP/TC, where TCP = Total Credit Point of that Semester TC =

Total Credit of that Semester

Cumulative Grade Point Average (CGPA) of a Programme is calculated using the formula

$$CGPA = \sum(TCP \times TC) \div \sum TC$$

CGPA shall be rounded off to two decimal places.

Grades for the different semesters and overall programme are given based on the corresponding CPA as shown below:

GPA	Grade
Equal to 9.5 and above	***S Outstanding***
Equal to 8.5 and below 9.5	***A+ Excellent***
Equal to 7.5 and below 8.5	***A Very Good***
Equal to 6.5 and below 7.5	***A- Good***
Equal to 5.5 and below 6.5	***B+ Above Average***
Equal to 5.0 and below 5.5	***B Average***
Equal to 4.0 and below 5.0	***C Pass***
Below 4.0	***F Failure***

M.Sc. PHARMACEUTICAL CHEMISTRY

	Code	Course	Hours/ week	Total Hours	Credit	Marks		
						Internal	External	Total
Semester 1	PG1PHA C01	Inorganic Chemistry-I (Coordination & Nuclear Chemistry)	4	72	4	20	80	100
	PG1PHA C02	Organic Chemistry-I (Structure, Reactivity & Stereochemistry)	4	72	4	20	80	100
	PG1PHA C03	Theoretical Chemistry-I (Quantum Chemistry and Group Theory)	4	72	4	20	80	100
	PG1PHA C04	Physical chemistry- I (Kinetic Theory, Thermodynamics and Statistical Thermodynamics)	3	54	3	20	80	100
	PG2PHA P01	Inorganic Chemistry Practical–1	3	54	Evaluation at the end of second semester			
	PG2PHA P02	Organic Chemistry Practical-1	3	54				
	PG2PHA P03	Physical Chemistry Practical -1	4	72				
		Total	**25**	**450**	**15**			
Semester 2	PG2PHA C05	Inorganic Chemistry-II (Bioinorganic & Organometallic Chemistry)	4	72	4	20	80	100
	PG2PHA C06	Organic Chemistry- II (Reaction Mechanism)	4	72	4	20	80	100
	PG2PHA C07	Theoretical Chemistry – II (Chemical Bonding and Computational Chemistry)	4	72	4	20	80	100
	PG2PHA C08	Physical chemistry- II (Molecular Spectroscopy)	3	54	3	20	80	100
	PG2PHA P01	Inorganic Chemistry Practical–1	3	54	3	20	80	100
	PG2PHA P02	Organic Chemistry Practical-1	3	54	3	20	80	100
	PG2PHA P03	Physical Chemistry Practical -1	4	72	3	20	80	100
		Total	**25**	**450**	**24**			

Semester 3	PG3PHA C09	Organic Chemistry- II (Synthetic and Bioorganic Chemistry)	4	72	4	20	80	100
	PG3PHA C10	Physical chemistry – III (Advanced Topics in Physical Chemistry)	4	72	4	20	80	100
	PG3PHA C11	Medicinal Chemistry- I (Drug Design and Pharmacologcy)	4	72	4	20	80	100
	PG3PHA C12	Spectroscopic Methods in Chemistry	3	54	3	20	80	100
	PG4PHA P04	Pharmaceutical Analysis and Pharmacognosy Practical	3	54	Evaluation at the end of fourth semester			
	PG4PHA P05	Drug Synthesis and Dispensing Practical	3	54				
	PG4PHA P06	Biochemistry and Bacteriology Practical	4	72				
		Total	**25**	**450**	**15**			
Semester 4	PG4PHA E01	Elective 1Bacteriology and Biochemistry	5	90	4	20	80	100
	PG4PHA E02	Elective 2 Pharmacognosy and Pharmaceutical Operations	5	90	4	20	80	100
	PG4PHA E03	Elective 3 Medicinal Chemistry- II	5	90	4	20	80	100
	PG4PHA E04	Elective 4 Polymer Chemistry	5	90	4	20	80	100
	PG4PHA E05	Elective 5 Analytical Chemistry	5	90	4	20	80	100
	PG4PHA P04	Pharmaceutical Analysis and Pharmacognosy Practical	3	54	3	20	80	100
	PG4PHA P05	Drug Synthesis and Dispensing Practical	3	54	3	20	80	100
	PG4PHA P06	Biochemistry and Bacteriology Practical	4	72	3	20	80	100
	PG4PHA D01	Project			2		100	100
	PG4PHA V01	Viva			2	20	80	100
		Total	**25**	**450**	**25**			
Grand Total					**80**			

SEMESTER 1

PG1PHA C01 INORGANIC CHEMISTRY – I

(COORDINATION & NUCLEAR CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Coordination Chemistry- Structural Aspects and Bonding (18 Hrs)

1.1 Classification of complexes based on coordination numbers and possible geometries. σ and π bonding ligands such as CO, NO, CN^-, R_3P and Ar_3P.

1.2 Splitting of *d* orbitals in octahedral, tetrahedral, square planar, square pyramidal and trigonal bipyramidal fields, LFSE, *Dq* values, Jahn Teller (JT) effect, theoretical failure of crystal field theory, evidence of covalency in the metal ligand bond, nephelauxetic effect, ligand field theory, molecular orbital theory- M.O energy level diagrams for octahedral and tetrahedral complexes with and without π-bonding, experimental evidences for π-bonding

Module 2: Kinetics and Mechanism of Reactions in Metal Complexes (18 Hrs)

2.1 Thermodynamic and kinetic stability, kinetics and mechanism of nucleophilic substitution reactions in square planar complexes, *trans* effect-theory and applications.

2.2 Kinetics and mechanism of octahedral substitution- water exchange, dissociative and associative mechanisms, base hydrolysis, racemization reactions, solvolytic reactions (acidic and basic).

2.3 Electron transfer reactions: outer sphere mechanism- Marcus theory, inner sphere mechanism-Taube mechanism.

Module 3: Organometallic Compounds- Synthesis, Structure and Bonding (18 Hrs)

3.1 Organometallic compounds with linear π- donor ligands- olefins, acetylenes, dienes and allyl complexes-synthesis, structure and bonding.

3.2 Complexes with cyclic π-donors- metallocenes and cyclic arene complexes structure and bonding. Hapto nomenclature. Carbene and carbyne complexes.

3.3 Preparation, properties, structure and bonding of simple mono and binuclear metal carbonyls, metal nitrosyls, metal cyanides and dinitrogen complexes. Polynuclear metal carbonyls

with and without bridging. Carbonyl clusters- LNCCS and HNCCS, Isoelectronic and isolobal analogy, Wade Mingos rules, cluster valence electrons.

Module 4: Electron deficient compounds (9 Hrs)

4.1. Electron deficient compounds – synthesis, reactions, structure and bonding. Boron hydrides, styx numbers, Boron cluster compounds. Wade's rule, Hydroborate anions, Organoboranes and hydroboration, Polyhedral anions, Carboranes, Metalloboranes, Borazines – Structure and bonding of borazines and Borides.

Module 5: Nuclear Chemistry (9 Hrs)

5.1 Fission products and fission yield. Neutron capture cross section and critical size. Nuclear fusion reactions and their applications. Chemical effects of nuclear transformations. Positron annihilation. Principles of counting technique such as G.M. counter, proportional, ionization and scintillation counters. Cloud chamber.

5.2 Synthesis of transuranic elements such as Neptunium, Plutonium, Curium, Berkelium, Einsteinium, Mendelevium, Nobelium, Lawrencium and elements with atomic numbers 104 to 109.

5.3 Analytical applications of radioisotopes- radiometric titrations, kinetics of exchange reactions, measurement of physical constants including diffusion constants, neutron activation analysis, prompt gamma neutron activation analysis and neutron absorptiometry.

5.4 Applications of radio isotopes in industry, medicine, autoradiography, radiopharmacology, radiation safety precaution, nuclear waste disposal.

5.5 Radiation chemistry of water and aqueous solutions- Fricke solution, Ceric ammonium solution. Measurement of radiation doses. Relevance of radiation chemistry in biology.

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[2] F.A. Cotton, G Wilkinson, C.A. Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th Edn., Wiley-Interscience, 1999.

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[4] P. Powell, Principles of Organometallic Chemistry, 2nd Edn., Chapman and Hall,1988.

[5] F. Basolo, R.G. Pearson, Mechanisms of Inorganic Reaction, John Wiley & Sons, 2006.

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PG1PHA C02 ORGANIC CHEMISTRY - I

(STRUCTURE, REACTIVITY & STEREOCHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: MO Theory and Aromaticity (9 Hrs)

1.1 Review of basic concepts in organic chemistry: bonding, hybridization, MO picture (allyl system, 1,3-butadiene and benzene), inductive effect, electromeric effect, resonance effect, hyperconjugation, steric effect. Bonding weaker than covalent bonds.

1.2 The formalism of curved arrow mechanisms. Practicing of line diagram drawing.

1.3 Concept of aromaticity: delocalization of electrons - Hückel's rule, criteria for aromaticity, examples of neutral and charged aromatic systems, azulenes, annulenes, mesoionic compounds. NMR as a tool for aromaticity. Antiaromatic and homoaromatic systems. Fullerenes, Carbon nanotubes and Graphene.

Module 2: Investigation of Organic Reaction Mechanisms (9 Hrs)

Energy profiles, Methods of determining reaction mechanisms, Kinetic and thermodynamic control of reactions. The Hammond postulate. Principle of microscopic reversibility. Marcus theory. The Hammett equation and its applications. Taft equation. Linear free energy relationships. Solvent polarity and parameters. Y, Z and E parameters and their applications. Primary and secondary kinetic isotope effects. Salt effects and special salt effects in SN reactions. Solvent effect. Bulk and specific solvent effects. Introduction to carbon acids - pKa of weak acids, kinetic and thermodynamic acidity. Phase transfer catalysis and its applications. Steric effects. HSAB principle and its applications in organic reactions.

Module 3: Review of Organic Reaction Mechanisms (18 Hrs)

3.1 Review of organic reaction mechanisms with special reference to nucleophilic and electrophilic substitution at aliphatic carbon (S_N1, S_N2, S_Ni, S_E1, S_E2), elimination (E1 and E2). Elimination vs substitution.

3.2 A comprehensive study on the effect of substrate, reagent, leaving group, solvent and neighbouring group on nucleophilic substitution (S_N2 and S_N1) and elimination (E1 and E2) reactions.

3.3 Addition reactions (regioselectivity- Markovnikov's addition- carbocation mechanism, anti-Markovnikov's addition- radical mechanism).

3.4 Mechanism of electrophilic and nucleophilic aromatic substitution reactions with examples. Arenium ion intermediates. S_N1, S_NAr, $S_{RN}1$ and Benzyne mechanisms.

3.5 Catalysis by acids, bases and nucleophiles with examples from acetal, cyanohydrin and ester formation and hydrolysis reactions- $A_{AC}2$, $A_{AC}1$, $A_{AL}1$, $B_{AC}2$ and $B_{AL}1$ mechanisms.

Module 4: Stereochemistry of Organic Compounds (18 Hrs)

4.1 Stereoisomerism: Definition based on symmetry and energy criteria. Projection formulae. Configurational isomerism. Geometrical isomerism- nomenclature, methods of determination of geometrical isomers based on physical properties, NMR spectroscopy and chemical methods. Optical isomerism, nomenclature.

4.2 Introduction to molecular symmetry and chirality: Examples from common objects to molecules. Axis, plane, center and alternating axis of symmetry.

4.3 Center of chirality: Molecules with C, N, S based chiral centers, absolute configuration, enantiomers, racemic modifications, R and S nomenclature using Cahn-Ingold-Prelog rules, molecules with a chiral center and C_n, molecules with more than one center of chirality, definition of diastereoisomers, constitutionally symmetrical and unsymmetrical chiral molecules, erythro and threo nomenclature.

4.4 Axial, planar and helical chirality with examples, stereochemistry and absolute configuration of allenes, biphenyls, binaphthyls, ansa and cyclophanic compounds, spiranes, exocyclic alkylidene cycloalkanes.

4.5 Topicity and prostereoisomerism, topicity of ligands and faces as well as their nomenclature. NMR distinction of enantiotopic/diastereotopic ligands.

4.6 Chiral drugs.

Module 5: Conformational Analysis (18 Hrs)

5.1 Conformational descriptors- factors affecting conformational stability of molecules. Conformational analysis of acyclic and cyclic systems: substituted ethanes, cyclohexane and its derivatives, decalins, adamantane, congressane, sucrose and lactose. Bridged bicyclic systems- norbornane, camphor, bicyclo[2.2.2]octane.

5.2. Conformation and reactivity of elimination (dehalogenation, dehydrohalogenation, semipinacolic deamination and pyrolytic elimination- Saytzeff and Hofmann eliminations), substitution and oxidation of 2° alcohols. Chemical consequence of conformational equilibrium - Curtin Hammett principle.

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PG1PHA C03 THEORETICAL CHEMISTRY – I

(QUANTUM CHEMISTRY AND GROUP THEORY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Formulation of Quantum Chemistry (18 Hrs)

1.1 Mathematical Concepts (5 Hrs)

Co-ordinate systems: Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. Complex numbers: definition, Complex conjugate, absolute value of a complex number, complex functions. Operator algebra: linear and nonlinear operators, Hermitian operators, del and del-squared operators. Eigen function and eigen values of an operator, Eigen value equation, Eigen functions of Commuting operators. Well behaved functions, Normalized and Orthogonal functions.

1.2 Evolution of Quantum Mechanics (5 Hrs)

Failure of classical mechanics: The black body radiation, Compton effect, photoelectric effect, atomic spectra. Need of quantum mechanics. Concept of matter wave, de Broglie relation and its experimental proof, Uncertainty principle and its consequences. Wave function and Born interpretation, Schrödinger's wave mechanics, Deduction of Schrodinger equation from classical wave equation.

1.3 Postulates of Quantum Mechanics (4 Hrs)

Detailed discussion of postulates: State function postulate. Operator postulate. Eigen value postulate. Expectation value postulate. Postulate of time dependent Schrodinger equation of motion, Conservative system and time-independent Schrodinger equation.

1.4 Quantum Mechanics of Translational Motion (4 Hrs)

Particle in one-dimension with infinite potential walls, particle in a three dimensional box-separation of variables- rectangular box and cubic box, degeneracy. Introduction to tunnelling with experimental evidence.

Module 2: Applications of Quantum Chemistry (18 Hrs)

2.1 Quantum Mechanics of Hydrogen-like Atoms (5 Hrs)

Potential energy of hydrogen-like systems. The wave equation in spherical polar coordinates: separation of variables- R, Θ and Φ equations and their solutions, wave functions and energies of hydrogen-like atoms. Orbitals- radial functions, radial distribution functions, angular functions and their plots.

2.2 Quantum Mechanics of Vibrational Motion (5 Hrs)

One-dimensional harmonic oscillator (complete treatment), Hermite equation (solving by method of power series), Hermite polynomials, recursion relation, wave functions and energies-important features, Harmonic oscillator model and molecular vibrations. Rodrigue's formula, Three dimensional harmonic oscillator.

2.3 Quantum Mechanics of Rotational Motion (5 Hrs)

Rotational motion: co-ordinate systems, Cartesian, Cylindrical polar and Spherical polar coordinates and their relationships. The wave equation in Spherical polar coordinates-particle on a ring, the Φ equation and its solution, wave functions in the real form. Non-planar rigid rotor (or particle on a sphere)-separation of variables, the Φ and the Θ equations and their solutions, Legendre and associated Legendre equations, Legendre and associated Legendre polynomials. Spherical harmonics (imaginary and real forms)- polar diagrams of spherical harmonics.

2.4 Orbital and Spin angular momentum (3 Hrs)

Quantisation of angular momentum, quantum mechanical operators corresponding to angular momenta, (L_x, L_y, L_z and L^2). Commutation relations between these operators. Spherical harmonics as eigen functions of angular momentum operators L_z and L^2. Space quantization. The postulate of spin by Uhlenbeck and Goudsmith, discovery of spin- Stern Gerlach experiment. Spin orbitals- construction of spin orbitals from orbital and spin functions.

Module 3: Molecular Symmetry and Mathematical group (18 Hrs)

3.1 Symmetry elements and symmetry operations. Conditions for a set of elements to form a group, sub groups, abelian and cyclic groups, Point groups. Multiplication of operations. Group multiplication table of C_{2v}, C_{2h} and C_{3v} groups (H_2O, Trans N_2F_2 and NH_3 as examples). Similarity transformation and classes in a group.

3.2 Matrices: addition and multiplication of matrices, inverse and orthogonal matrices, character of a matrix, block diagonalisation, matrix representation of symmetry operations, representation of groups by matrices, construction of representation using vectors and atomic

orbitals as basis, representation generated by Cartesian coordinates positioned on the atoms of a molecule (H_2O as example).

3.3 Reducible and Irreducible representations (IR). Reduction formula, reduction of reducible representation to IRs.

Module 4: Applications of Group Theory (18 Hrs)

4.1 The Great Orthogonality theorem. Rules derived from GOT (proof not required). Setting up of character table of C_{2v}, C_{3v}, C_{2h}, C_{4v} and C_3 groups. Direct product representations.

4.2 Applications in quantum mechanics, transition moment integral, vanishing of integrals. Jahn – Teller effect, Woodward – Hoffmann rules.

4.3 Applications in vibrational spectra: symmetry aspects of molecular vibrations, vibrations of polyatomic molecules-selection rules for vibrational absorption. Determination of the symmetry of normal modes of H_2O, Trans-N_2F_2 and NH_3 using Cartesian coordinates and internal coordinates. Complementary character of IR and Raman spectra- determination of the number of active IR and Raman lines.

4.4 Application in electronic spectra: selection rules for electronic transition, electronic transitions due to the carbonyl chromophore in formaldehyde.

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PG1PHA C04 - PHYSICAL CHEMISTRY - I

(KINETIC THEORY, THERMODYNAMICS AND STATISTICAL THERMODYNAMICS)

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Kinetic theory (9 Hrs)

Kinetic theory of gases, derivation of Maxwell's law of distribution of velocities, graphical representation, experimental verification of the law, most probable velocity, derivation of average, RMS and most probable velocities, collision diameter, collision frequency in a single gas and in a mixture of two gases, mean free path, frequency of collision, effusion, the rate of effusion, time dependence of pressure of an effusing gas, transport properties of gases. Viscosity, thermal conductivity and diffusion. Determination of viscosity of gases. Influence of temperature and pressure on transport properties.

Module 2: Classical Thermodynamics (18 Hrs)

2.1 Entropy, dependence of entropy on variables of a system (S, T and V; S, T and P). Thermodynamic equations of state. Irreversible processes - Clausius inequality.

2.2 Free energy, Maxwell relations and significance, temperature dependence of free energy, Gibbs-Helmholtz equation, applications of Gibbs-Helmholtz equation.

2.3 Partial molar quantities, chemical potential and Gibbs-Duhem equations, determination of partial molar volume and enthalpy.

2.4 Fugacity, relation between fugacity and pressure, determination of fugacity of a real gas, variation of fugacity with temperature and pressure. Activity, dependence of activity on temperature and pressure.

2.5 Thermodynamics of mixing, Gibbs-Duhem-Margules equation, Konowaloff's rule, Henry's law, excess thermodynamic functions- free energy, enthalpy, entropy andvolume. Determination of excess enthalpy and volume.

2.6 Chemical affinity and thermodynamic functions, effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherm.

2.7 Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, entropy changes in chemical reactions.

2.8 Three component systems- graphical representation. solid-liquid equilibria- ternary solutions with common ions, hydrate formation, compound formation. Liquid-liquid equilibria- one pair of partially miscible liquids, two pairs of partially miscible liquids, and three pairs of partially miscible liquids.

Module 3: Irreversible Thermodynamics and Bioenergetics (9 Hrs)

3.1 Thermodynamics of irreversible processes with simple examples. Uncompensated heat and its physical significance. Entropy production- rate of entropy production, entropy production in chemical reactions, the phenomenological relations, the principle of microscopic reversibility, the Onsager reciprocal relations thermal osmosis, thermoelectric phenomena.

3. 2 Bioenergetics: Coupled reactions, ATP and its role in bioenergetics, high energy bond, free energy and entropy change in ATP hydrolysis, thermodynamic aspects of metabolism and respiration, glycolysis, biological redox reactions.

Module 4: Statistical Thermodynamics (18 Hrs)

4.1 Permutation, probability, apriori and thermodynamic probability, Stirling's approximation, macrostates and microstates, Boltzmann distribution law, partition function and its physical significance, phase space, different ensembles, canonical partition function, distinguishable and indistinguishable molecules, partition function and thermodynamic functions, separation of partition function- translational, rotational, vibrational and electronic partition functions. Thermal de-Broglie wavelength.

4.2 Calculation of thermodynamic functions and equilibrium constants, statistical interpretation of work and heat, Sakur-Tetrode equation, statistical formulation of third law of thermodynamics, thermodynamic probability and entropy, residual entropy, heat capacity of gases - classical and quantum theories, heat capacity of hydrogen.

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[1] P.W. Atkins, Physical Chemistry, ELBS, 1994.

[2] K.J. Laidler, J.H. Meiser, B.C. Sanctuary, Physical Chemistry, 4th Edn., Houghton Mifflin, 2003.

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SEMESTER 2

PG2PHA C05 INORGANIC CHEMISTRY- II

(BIOINORGANIC & ORGANOMETALLIC CHEMISTRY)

Credits: 4 **Contact Lecture Hours: 72**

Module 1: Bioinorganic Compounds (18 Hrs)

1.1 Essential and trace elements in biological systems, structure and functions of biological membranes, mechanism of ion transport across membranes, sodium pump, ionophores, valinomycin and crown ether complexes of Na^+ and K^+, ATP and ADP. Photosynthesis- chlorophyll a, PS I and PS II. Role of calcium in muscle contraction, blood clotting mechanism and biological calcification.

1.2 Oxygen carriers and oxygen transport proteins- haemoglobins, myoglobins and haemocyanin, haemerythrins and haemevanadins, cooperativity in haemoglobin. Iron storage and transport in biological systems- ferritin and transferrin. Redox metalloenzymes-cytochromes, peroxidases and superoxide dismutase and catalases. Nonredox metalloenzymes- Carboxypeptidase A- structure and functions. Nitrogen fixation- nitrogenase, vitamin B_{12} and vitamin B_{12} coenzymes.

1.3 Metals in medicine- therapeutic applications of *cis*-platin, radio-isotopes and MRI agents. Toxic effects of metals (Cd, Hg, Cr and Pb).

Module 2: Inorganic Chains (9 Hrs)

2.1 Chains - catenation, homo and heterocatenation. Silicate minerals. Structure of silicates common silicates, silicates containing discrete anions, silicates containing infinite chains, silicates containing sheets, framework silicates. Silicones. Zeolites synthesis, structure and applications. Isopoly acids of vanadium, molybdenum and tungsten. Heteropoly acids of Mo and W. Condensed phosphates-preparation, structure and applications. Phosphate esters in biological systems. Polythiazil- one dimensional conductors.

Module 3: Spectral and Magnetic Properties of Metal Complexes (18 Hrs)

3.1 Electronic Spectra of complexes- Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition- effect of spin orbit coupling and vibronic coupling.

3.2 Interpretation of electronic spectra of complexes- Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of *Dq*, *B* and β (Nephelauxetic ratio) values, spectra of complexes with lower symmetries, charge transfer spectra, luminescence spectra.

3.3 Magnetic properties of complexes- paramagnetic and diamagnetic complexes, molar susceptibility, Gouy method for the determination of magnetic moment of complexes, spin only magnetic moment. Temperature dependence of magnetism- Curie's law, Curie-Weiss law. Temperature Independent Paramagnetism (TIP), Spin state cross over, Antiferromagnetism- inter and intra molecular interaction. Anomalous magnetic moments.

3.4 Elucidating the structure of metal complexes (cobalt and nickel complexes) using electronic spectra, IR spectra and magnetic moments.

Module 4: Stereochemistry of Coordination Compounds (9 Hrs)

4.1 Geometrical and optical isomerism in octahedral complexes, resolution of optically active complexes, determination of absolute configuration of complexes by ORD and circular dichroism, stereoselectivity and conformation of chelate rings, asymmetric synthesis catalyzed by coordination compounds.

4.2 Linkage isomerism- electronic and steric factors affecting linkage isomerism. Symbiosis- hard and soft ligands, Prussian blue and related structures, Macrocycles- crown ethers.

Module 5: Reactions of Organometallic Compounds (9 Hrs)

5.1 Substitution reactions- nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.

5.2 Addition and elimination reactions- 1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.

5.3 Rearrangement reactions, redistribution reactions, fluxional isomerism.

Module 6: Catalysis of Organometallic Compounds (9 Hrs)

6.1 Alkene hydrogenation, Tolman catalytic loop, Synthesis gas, Hydroformylation, Monsanto Acetic acid process, Wacker process, Zeigler Natta catalysis.

References

[1] F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry: A Comprehensive Text, 3rd Edn., Interscience,1972.

[2] J.E. Huheey, E.A. Keiter, R.A. Keiter, Inorganic Chemistry Principles of Structure and Reactivity, 4th Edn., Pearson Education India, 2006.

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PG2PHA C06 ORGANIC CHEMISTRY - II

(REACTION MECHANISM)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Chemistry of Carbocations (9 Hrs)

1.1 Formation, structure and stability of carbocations. Classical and non-classical carbocations.

1.2 C-X bond (X = C, O, N) formations through the intermediary of carbocations. Molecular rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol, Dienone-phenol and Benzilic acid rearrangements, Prins reaction, Demjanov rearrangement. Oxymercuration, halolactonisation.

Module 2: Chemistry of Carbanions (18 Hrs)

2.1 Formation, structure and stability of carbanions. Reactions of carbanions: C-X bond (X = C, O, N) formations through the intermediary of carbanions. Chemistry of enolates, Kinetic and thermodynamic enolates- Lithium and boron enolates in Michael and aldol reactions, alkylation and acylation of enolates. Chemistry of enamines, Stork-Enamine reaction.

2.2 Nucleophilic additions to carbonyls groups. Reactions involving carbanions- mechanisms of Claisen, Dieckmann, Knoevenagel, Stobbe, Darzen and acyloin condensations, Shapiro reaction and Julia elimination. Favorskii rearrangement.

2.3 Reactions of carbonyl compounds: oxidation, reduction (Clemmensen and Wolff-Kishner), addition reactions (addition of cyanide, ammonia, alcohol), Aldol condensation, Cannizzaro reaction, addition of Grignard reagent.

2.4 Structure and reactions of α, β- unsaturated carbonyl compounds involving electrophilic and nucleophilic addition- Michael addition, Mannich reaction, Robinson annulation.

2.5 Ylids: chemistry of phosphorous and sulphur ylids - Wittig and related reactions, Peterson olefination.

Module 3: Carbenes, Carbenoids, Nitrenes and Arynes (9 Hrs)

3.1 Generation, structure and reactions of carbenes. Rearrangement reactions of carbenes: Wolff rearrangement, generation and reactions of ylids by carbenoid decomposition.

3.2 Structure, generation and reactions of nitrenes. Hoffmann, Curtius, Lossen, Schmidt and Beckmann rearrangement reactions.

3.3 Arynes: generation, structure, stability and reactions. Orientation effect, amination of haloarenes.

Module 4: Radical Reactions (9 Hrs)

4.1 Generation and detection of radical intermediates and its (a) addition to alkenes, alkynes (inter and intramolecular) for C-C bond formation - Baldwin's rules (b) fragmentation and rearrangements. Hydroperoxide: formation, rearrangement and reactions. Autoxidation.

4.2 Name reactions involving radical intermediates: Barton deoxygenation and decarboxylation, McMurry coupling.

Module 5: Concerted reactions (18 Hrs)

5.1 Symmetry properties of molecular orbitals of ethylene and conjugated systems with three or more atoms, Woodward – Hoffmann rule, Conservation of orbital symmetry and stereo chemical courses.

5.2 Pericyclic reactions like Electrocyclic (butadiene-cyclobutene and hexatriene-cyclohexadiene interconversions), Cycloadditions (2+2) & (4+2), Sigmatropic (1,3), (1,5) and (3,3), Cheletropic including Cheletropic eliminations and Ene reaction with stereo chemical aspects.

5.3 Diels- Alder reactions with stereochemical aspects.

5.4 Analysis of Pericyclic Reactions. (i) FMO method (ii) Orbital- correlation method and (iii) PMO method.

5.2 Highlighting pericyclic reactions in organic synthesis such as Claisen, Cope, Mislow-Evans, Wittig and Sommelet-Hauser rearrangements. dipolar cycloaddition (introductory). Unimolecular pyrolytic elimination reactions, decomposition of cyclic azo compounds, β-eliminations involving cyclic transition states such as N-oxides, acetates and xanthates.

Module 6: Organic Photochemistry (9 Hrs)

6.1 Photochemical processes. Energy transfer. Jablonski diagram, sensitization and quenching. Singlet and triplet states and their reactivity.

6.2 Photoreactions of carbonyl compounds, enes, dienes and arenes. Norrish reactions of acyclic ketones. Patterno-Buchi, Barton, Photo-Fries and Di-л methane rearrangements. Photoreactions of Vitamin D. Photosynthesis and photochemistry of vision. Singlet oxygen generation and their reactions**.**

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[1] R. Bruckner, Advanced Organic Chemistry: Reaction Mechanism, Academic Press, 2002.

[2] F.A. Carey, R.A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edn., Springer Science & Business Media, 2007.

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PG2PHA C07 THEORETICAL CHEMISTRY - II

(CHEMICAL BONDING AND COMPUTATIONAL CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Approximate Methods in Quantum Mechanics (18 Hrs)

1.1 Many-body problem and the need of approximation methods, independent particle model. Variation method, variation theorem with proof, illustration of variation theorem using the trial function x(a-x) for particle in a 1D – box and using the trial function e^{-ar} for the hydrogen atom, variation treatment for the ground state of helium atom.

1.2 Perturbation method, time-independent perturbation method (non-degenerate case only), first order correction to energy and wave function, illustration by application to particle in a 1D-box with slanted bottom, perturbation treatment of the ground state of the helium atom. Qualitative idea of Hellmann-Feynman theorem.

1.3 Hartree Self-Consistent Field method. Spin orbitals for many electron atoms- symmetric and antisymmetric wave functions. Pauli's exclusion principle. Slater determinants. Qualitative treatment of Hartree-Fock Self-Consistent Field (HFSCF) method. Roothan's concept of basis functions, Slater type orbitals (STO) and Gaussian type orbitals (GTO), sketches of STO and GTO.

Module 2: Chemical Bonding (18 Hrs)

2.1 Schrödinger equation for molecules. Born-Oppenheimer approximation. Valence Bond (VB) theory, VB theory of H_2 molecule, singlet and triplet state functions (spin orbitals) of H_2.

2.2 Molecular Orbital (MO) theory, MO theory of H_2^+ ion, MO theory of H_2 molecule, MO treatment of homonuclear diatomic molecules Li_2, Be_2, N_2, O_2 and F_2 and hetero nuclear diatomic molecules LiH, CO, NO and HF. Bond order. Spectroscopic term symbols for diatomic molecules. Comparison of MO and VB theories.

2.3 Hybridization, quantum mechanical treatment of sp, sp^2 and sp^3 hybridisation. Semiempirical MO treatment of planar conjugated molecules, Hückel Molecular Orbital (HMO) theory of ethene, allyl systems, butadiene and benzene. Calculation of charge distributions, bond order and free valency.

Module 3: Applications of Group Theory in Chemical Bonding (9 Hrs)

3.1 Applications in chemical bonding, construction of hybrid orbitals with BF_3, CH_4, and PCl_5 as examples. Transformation properties of atomic orbitals. Symmetry adapted linear combinations (SALC) of C_{2v}, C_{3v}, C_{2h}, C_3 and D_{3h} groups. MO diagram for water and ammonia.

Module 4: Computational Chemistry (18 Hrs)

4.1 Introduction: computational chemistry as a tool and its scope.

4.2 Potential energy surface: stationary point, transition state or saddle point, local and global minima.

4.3 Molecular mechanics methods: force fields-bond stretching, angle bending, torsional terms, non-bonded interactions, electrostatic interactions. Mathematical expressions. Parameterisation from experiments of quantum chemistry. Important features of commonly used force fields like MM3, MMFF, AMBER and CHARMM.

4.4 Ab initio methods: A review of Hartee-Fock method. Basis set approximation. Slater and Gaussian functions. Classification of basis sets - minimal, double zeta, triple zeta, split valence, polarization and diffuse basis sets, contracted basis sets, Pople style basis sets and their nomenclature, correlation consistent basis sets.

4.5 Hartree-Fock limit. Electron correlation. Qualitative ideas on post Hartree-Fock methods-variational method, basic principles of Configuration Interaction (CI). Perturbational methods-basic principles of Møller Plesset Perturbation Theory.

4.6 General introduction to semiempirical methods: basic principles and terminology.

4.7 Introduction to Density Functional Theory (DFT) methods: Hohenberg-Kohn theorems. Kohn-Sham orbitals. Exchange correlation functional. Local density approximation. Generalized gradient approximation. Hybrid functionals (only the basic principles and terms need to be introduced).

4.8 Model Chemistry-notation, effect on calculation time (cost).

4.9 Comparison of molecular mechanics, ab initio, semiempirical and DFT methods

Module 5: Computational Chemistry Calculations (9 Hrs)

5.1 Molecular geometry input- Cartesian coordinates and internal coordinates, Z-matrix. Z-matrix of: single atom, diatomic molecule, non-linear triatomic molecule, linear triatomic molecule, polyatomic molecules like ammonia, methane, ethane and butane. General format of GAMESS/Firefly input file. GAMESS/Firefly key word for: basis set selection, method selection, charge, multiplicity, single point energy calculation, geometry optimization, constrained optimization and frequency calculation.

5.2 Identifying a successful GAMESS/Firefly calculation-locating local minima and saddle points, characterizing transition states, calculation of ionization energies, Koopmans' theorem, electron affinities and atomic charges.

5.3 Identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations using suitable graphics packages.

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[1] I.N. Levine, Quantum Chemistry, 6th Edn., Pearson Education, 2009.

[2] D.A. McQuarrie, Quantum Chemistry, University Science Books, 2008.

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Softwares

Molecular Mechanics:

01. **Arguslab** available from www.arguslab.com/
02. **Tinker** available from www.dasher.wustl.edu/ffe/

Ab initio, semiempirical and dft:

01. **Firefly / PC GAMESS** available from http://classic.chem.msu.su/gran/gamess/
02. **WINGAMESS** available from http://www.msg.ameslab.gov/gamess/

Graphical User Interface (GUI):

01. **Gabedit** available from http://gabedit.sourceforge.net/
02. **wxMacMolPlt** available from http://www.scl.ameslab.gov/MacMolPlt/
03. **Avogadro** from http://avogadro.openmolecules.net/wiki/Get_Avogadro

PG2 PHA C08 PHYSICAL CHEMISTRY - II

(MOLECULAR SPECTROSCOPY)

Credit: 3 **Contact Lecture Hours: 54**

Module 1: Microwave and Infrared Spectroscopy (18 Hrs)

1.1 Origin of spectra: origin of different spectra and the regions of the electromagnetic spectrum, intensity of absorption, influencing factors, signal to noise ratio, natural line width-contributing factors, Lamb dip spectrum, Born Oppenheimer approximation, energy dissipation from excited states (radiative and non-radiative processes), relaxation time.

1.2 Microwave spectroscopy: principal moments of inertia and classification of molecules (linear, symmetric tops, spherical tops and asymmetric tops), selection rules, intensity of rotational lines, relative population of energy levels, derivation of J_{max}, effect of isotopic substitution, calculation of intermolecular distance, spectrum of non rigid rotors, rotational spectra of polyatomic molecules, linear and symmetric top molecules, Stark effect and its application, nuclear spin and electron spin interaction, chemical analysis by microwave spectroscopy.

1.3 Infrared spectroscopy: Morse potential energy diagram, fundamentals, overtones and hot bands, determination of force constants, diatomic vibrating rotator, break down of the Born-Oppenheimer approximation, effect of nuclear spin, vibrational spectra of polyatomic molecules, normal modes of vibrations, combination and difference bands, Fermi resonance, finger print region and group vibrations, effect of H-bonding on group frequency, disadvantages of dispersive IR, introduction to FT spectroscopy, FTIR.

Module 2: Electronic, Mossbauer and Raman spectroscopy (18 Hrs)

2.1 Electronic spectroscopy: Term symbols of diatomic molecules, electronic spectra of diatomic molecules, selection rules, vibrational coarse structure and rotational fine structure of electronic spectrum, Franck-Condon principle, predissociation, calculation of heat of dissociation, Birge and Sponer method, electronic spectra of polyatomic molecules, spectra of transitions localized in a bond or group, free electron model.

Different types of lasers- solid state lasers, continuous wave lasers, gas lasers and chemical laser, frequency doubling, applications of lasers, introduction to UV and X-ray photoelectron spectroscopy.

2.2 Mossbauer spectroscopy: principle, Doppler effect, recording of spectrum, chemical shift, factors determining chemical shift, application to metal complexes, MB spectra of Fe(II) and Fe(III) cyanides.

2.3 Raman spectroscopy: scattering of light, polarizability and classical theory of Raman spectrum, rotational and vibrational Raman spectrum, complementarities of Raman and IR spectra, mutual exclusion principle, polarized and depolarized Raman lines, resonance Raman scattering and resonance fluorescence.

Module 3: Resonance Spectroscopy (18 Hrs)

3.1 NMR spectroscopy : Interaction between nuclear spin and applied magnetic field, nuclear energy levels, population of energy levels, Larmor precession, relaxation methods, chemical shift, representation, examples of AB, AX and AMX types, exchange phenomenon, factors influencing coupling, Karplus relationship.

3.2 FTNMR, second order effects on spectra, spin systems (AB, AB_2), simplification of second order spectra, chemical shift reagents, high field NMR, double irradiation, selective decoupling, double resonance, NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR, natural abundance, sensitivity, ^{13}C chemical shift and structure correlation, introduction to solid state NMR, magic angle spinning.

3.3 EPR spectroscopy: electron spin in molecules, interaction with magnetic field, g factor, factors affecting g values, determination of g values ($g_{\parallel}$ and $g_{\perp}$), fine structure and hyperfine structure, Kramers' degeneracy, McConnell equation.

3.4 An elementary study of NQR spectroscopy.

References

[1] C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., Tata McGraw Hill, 1994.

[2] G. Aruldhas, Molecular Structure and Spectroscopy, Prentice Hall of India, 2001.

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SEMESTERS 1 AND 2

PG2 PHA P01 INORGANIC CHEMISTRY PRACTICAL – 1

Credit: 3 **Contact Lab Hours: 54 + 54 = 108**

PART I

Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li and common cations - Ag^{+}, Hg^{2+}, Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, As^{3+}, Sn^{2+}, Sb^{3+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+} (interfering acid radicals are not present). Confirmation by spot test (Minimum **8** mixtures are to be recorded).

PART II

1. Argentometric estimation of chlorides
2. Cerimetry – Fe(II) and nitrate
3. Potassium iodate – iodide estimation of Sn(II)

PART III

Colorimetric estimation of Cr, Fe, Ni, Mn, Cu, NH_4^{+}, nitrate and phosphate ions.

PART IV

Preparation and characterization of complexes using IR, NMR and electronic spectra.

1. Tris (thiourea) copper (I) complex
2. Potassium tris (oxalate) aluminate (III)
3. Tetrammine copper (II) sulphate
4. Mercury tetra thiocyanato cobaltate (III)

References

[1] A.I. Vogel, A Text Book of Qualitative Inorganic Analysis Including Elementary Instrumental Analysis, 3rd Edn., ELBS.
[2] G. Svelha, Text Book of Vogel's Macro and Semi-micro Inorganic Analysis, revised, Orient Longman.
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PG2 PHA P02 ORGANIC CHEMISTRY PRACTICAL - 1

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

General methods of separation and purification of organic compounds such as:

1. Solvent extraction
2. Soxhlet extraction
3. Fractional crystallization
4. TLC and Paper Chromatography
5. Column Chromatography
6. Membrane Dialysis

PART II

A. Separation of organic binary mixtures:- 1. Quantitative separation of a mixture of two components by solvent extraction 2. Purification of the separated samples by distilling and crystallization. 3. Determination of physical constants of separated and purified samples (No need of bifunctional compounds).

B. Separation of organic mixtures by TLC and calculation of R_f values.

C. Separation/purification of organic mixtures by column chromatography.

PART III

Drawing the structures of organic molecules and reaction schemes and mechanisms by ChemDraw, SymyxDraw and Chemsketch.

1. Cycloaddition of diene and dienophile (Diels-Alder reaction).
2. Oxidation of primary alcohol to aldehyde and then to acid.
3. Benzoin condensation.
4. Esterification of simple carboxylic acids.
5. Aldol condensation.

PART IV- Viva voce

References

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[4] R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

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[7] N.K.Vishnoi, Advanced Practical Organic Chemistry, 3rd Edn., Vikas Publishing House, 2009.

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PG2 PHA P03 PHYSICAL CHEMISTRY PRACTICAL - 1

Credit: 3 **Contact Lab Hours: 72+72 =144**

(One question each from both parts A and B will be asked for the examination)

Part A

I. Adsorption

1. Verification of Freundlich and Langmuir adsorption isotherm: charcoal-acetic acid or charcoal-oxalic acid system.
2. Determination of the concentration of the given acid using the isotherms.

II. Phase diagrams

1. Construction of phase diagrams of simple eutectics.
2. Construction of phase diagram of compounds with congruent melting point: diphenyl amine-benzophenone system.
3. Effect of (KCl/succinic acid) on miscibility temperature.
4. Construction of phase diagrams of three component systems with one pair of partially miscible liquids.

III. Distribution law

1. Distribution coefficient of iodine between an organic solvent and water.
2. Distribution coefficient of benzoic acid between benzene and water.
3. Determination of the equilibrium constant of the reaction $KI + I_2 \leftrightarrow KI_3$

IV. Surface tension

1. Determination of the surface tension of a liquid by
   a) Capillary rise method
   b) Drop number method
   c) Drop weight method
2. Determination of parachor values.

3. Determination of the composition of two liquids by surface tension measurements.

Part B

Computational Chemistry Experiments

V. Experiments illustrating the capabilities of modern open source/free computational chemistry packages in computing single point energy, geometry optimization, vibrational frequencies, population analysis, conformational studies, IR and Raman spectra, transition state search, molecular orbitals, dipole moments etc.

Geometry input using Z-matrix for simple systems, obtaining Cartesian coordinates from structure drawing programs like Chemsketch.

References

[1] J.B. Yadav, Advanced Practical Physical Chemistry, Goel Publishing House, 2001.

[2] G.W. Garland, J.W. Nibler, D.P. Shoemaker, Experiments in Physical Chemistry, 8th Edn., McGraw Hill, 2009.

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SEMESTER 3

PG3PHA C09 ORGANIC CHEMISTRY- III

(SYNTHETIC AND BIOORGANIC CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Organic Synthesis via Oxidation and Reduction (18 Hrs)

1.1 Survey of organic reagents and reactions in organic chemistry with special reference to oxidation. Metal based and non-metal based oxidations of (a) alcohols to carbonyls (chromium, manganese, aluminium, and silver based reagents) (b) phenols (Fremy's salt, silver carbonate) (c) alkenes to epoxides (peroxides/peracids based), Sharpless asymmetric epoxidation (d) alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction (e) alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based, ozonolysis) (f) alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation) (g) ketones to ester/lactones (Baeyer-Villiger).

1.2 Survey of organic reagents and reactions in organic chemistry with special reference to reduction (a) Catalytic hydrogenation (Heterogeneous: Pd /Pt /Rh /Ni; Homogeneous: Wilkinson), Noyori asymmetric hydrogenation (b) Metal based reductions using Li/Na/Ca in liquid ammonia, Sodium, Magnesium and Zinc (Birch, Pinacol formation, McMurry, Acyloin formation, dehalogenation and deoxygenations) (c) Hydride transfer reagents from Group III and Group IV in reductions (i) $NaBH_4$, triacetoxyborohydride; $LiAlH_4$ and DIBAL-H, Meerwein-Pondorff-Verley reduction) (ii) Stereo/enantioselective reductions (Chiral boranes, Corey-Bakshi-Shibata).

Module 2: Modern Synthetic Methods (9 Hrs)

2.1 Baylis-Hillman reaction, Henry reaction, Nef reaction, Sakurai reaction, Tishchenko reaction. Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi, Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann and Glaser coupling reactions. Reagents such as: NBS, DDQ, DCC, Gilman reagent.

2.2 Introduction to multicomponent reactions- Three component reactions (Mannich reaction, Passerini reaction, Biginelli reaction), Four component reactions (Ugi reaction). Click reactions (Elementary idea only).

Module 3: Stereoselective Transformations (9 Hrs)

3.1 Asymmetric induction-chiral auxiliaries and chiral pool.

3.2 Enantioselective catalytic hydrogenation developed by Noyori and Knowels.

3.3 Asymmetric aldol condensation pioneered by Evans.

3.4 Asymmetric Diels-Alder reactions.

3.5 Asymmetric epoxidation using Jacobsen's catalyst.

Module 4: Construction of Ring Systems (9 Hrs)

4.1 Different approaches towards the synthesis of three, four, five and six-membered rings-Pauson-Khand reaction, Bergman cyclization, Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization. Ring closing metathesis.

4.2 Structure and formation of heterocyclic rings: 5-and 6-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O- pyrrole, furan, thiophene, imidazole, pyrazole, thiazole, oxazole, pyridine, purines and pyrimidines, quinoline and isoquinoline.

Module 5: Molecular Recognition and Supramolecular Chemistry (9 Hrs)

5.1 Concept of molecular recognition, host-guest complex formation, Forces involved in molecular recognition.

5.2 Molecular receptors: Cyclodextrins, Crown ethers, Cryptands, Tweezers, Carcerands, Cyclophanes, Calixaranes, carbon nanocapsules.

5.3 Importance of molecular recognition in biological systems.

5.4 Applications of supramolecular complexes in medicine and perfumery industries.

Module 6: Chemistry of Natural Products and Biomolecules (18 Hrs)

6.1 Terpenoids: Classification of terpenoids. Synthesis of camphor. Biogenesis of isoprenoids.

6.2 Steroids: classification and nomenclature of steroids. Reactions, structure elucidation, stereochemistry and biosynthesis of cholesterol. Structure and semi synthesis of steroid hormones-testosterone, estrogen and progesterone. Biosynthesis of steroids.

6.3 Alkaloids: Classification of alkaloids, general methods of structure elucidation of alkaloids. Structure elucidation and synthesis of papaverine, quinine and morphine. Stereoselective synthesis of reserpine. Biosynthesis of alkaloids- papaverine, morphine.

6.4 Vitamins: classification and structure of vitamins A, B_1, B_2, B_6, and C. Synthesis of vitamins A, C, B_1 and B_2.

6.5 Natural colouring species: anthocyanins and carotenoids, structure and synthesis of cyanin, flavone, quercetine and β-carotene.

6.6 Basic principles of the biosynthesis of terpenes, carbohydrates, proteins and nucleic acids. Biomimetic synthesis of progesterone and spatriene.

References

[1] F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2009.

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[19] V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, CRS Press, 2007.

[20] P. S. Kalsi, Sangeeta Jagtap, Pharmaceutical, Medicinal and Natural Product Chemistry, Alpha Science, 2013

PG3PHA C10 PHYSICAL CHEMISTRY- III

(ADVANCED TOPICS IN PHYSICAL CHEMISTRY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Electrochemistry and Electromotive Force (9 Hrs)

1.1 Theories of ions in solution, Drude and Nernst's electrostriction model and Born's model, Debye-Huckel theory, Derivation of Debye-Huckel-Onsager equation, validity of DHO equation for aqueous and non aqueous solutions, Debye- Falkenhagen effect, conductance with high potential gradients, activity and activity coefficients in electrolytic solutions, ionic strength, Debye-Huckel limiting law and its various forms, qualitative and quantitative tests of Debye-Huckel limiting equation, deviations from the DHLL.

Module 2: Chemical Kinetics (18 Hrs)

2.1 Theories of reaction rates: Collision theory-steric factor, potential energy surfaces. Conventional transition state theory- Eyring equation. Comparison of the two theories.Thermodynamic formulation of the two theories. Thermodynamic formulation of the reaction rates. Significance of $\Delta G^{\#}$, $\Delta H^{\#}$ and $\Delta S^{\#}$. Volume of activation. Effect of pressure and volume on velocity of gas reactions.

2.2 Lindemann-Hinshelwood mechanism and RRKM theory of unimolecular reactions. Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, cage effect, Bronsted-Bjerrum equation, primary and secondary kinetic salt effect, influence of solvent on reaction rates, significance of volume of activation, Hammet and Taft equation, kinetic isotope effect.

2.3 Fast reactions: relaxation, flow and shock methods, flash photolysis, NMR and ESR methods of studying fast reactions.

Module 3: Surface Chemistry and Colloids (18 Hrs)

3.1 Different types of surfaces, thermodynamics of surfaces, Gibbs adsorption equation and its verification, surfactants and micelles, general properties of emulsions, foam structure, aerosols, surface films, surface pressure and surface potential and their measurements and interpretation. Application of low energy electron diffraction and photoelectron spectroscopy, ESCA and Auger

electron spectroscopy, scanning probe microscopy, ion scattering, SEM and TEM in the study of surfaces.

3.2 Adsorption: The Langmuir theory, kinetic and statistical derivation, multilayer adsorption-BET theory, Use of Langmuir and BET isotherms for surface area determination. Application of Langmuir adsorption isotherm in surface catalysed reactions, the Eley-Rideal mechanism and the Langmuir-Hinshelwood mechanism, flash desorption.

3.3 Colloids: Zeta potential, electrokinetic phenomena, sedimentation potential and streaming potential, Donnan membrane equilibrium.

Module 4: Quantum Statistics (9 Hrs)

4.1 Need for quantum statistics, Bose-Einstein statistics: Bose-Einstein distribution, example of particles, Bose-Einstein condensation, difference between first order and higher order phase transitions, liquid helium, supercooled liquids. Fermi- Dirac distribution: examples of particles, application in electron gas, thermionic emission. Comparison of three statistics- Maxwell Boltzmann, Bose Einstein and Fermi - Dirac Statistics.

4.2 Heat capacity of solids- Dulong and Petit's law, the vibrational properties of solids, Einsteins theory- Derivation, and its limitations, Debye theory – derivation and its limitations.

Module 5: Photochemistry (18 Hrs)

5.1 Quantum yield, chemical actinometry, excimers and exciplexes, photosensitization, chemiluminescence, bioluminescence, thermoluminescence, pulse radiolysis, hydrated electrons, photostationary state, dimerisation of anthracene, ozone layer in the atmosphere, chemistry of photosynthesis, photography and vision.

5.2 Principle of utilization of solar energy, solar cells and their working.

5.3 Quenching of fluorescence and its kinetics, Stern-Volmer equation, concentration quenching, fluorescence and structure, delayed fluorescence, E-type and P-type, effect of temperature on emissions, photochemistry of environment, green house effect, two photon absorption spectroscopy, application of pulsed laser in measuring the dynamics of photochemical processes. Photochemistry of vision. Phototaxis and phototropism. Photochemistry of nucleic acids. Vitamin D.

References

[1] J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.

[2] K. J. Laidler, Chemical Kinetics, 3rd Edn., Harper & Row, 1987.

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PG3PHA C11 MEDICINAL CHEMISTRY – I

(DRUG DESIGN & PHARMACOLOGY)

Credit: 4 **Contact Lecture Hours: 72**

Module 1: Drug Discovery, Design and Development (27 Hrs)

1.1 Development of new drugs: Lead discovery, Random screening, rational approaches, sources of lead compounds, methods of lead discovery, lead modification, identification of pharmacophore, functional group modification, structure-activity relationships, drug-like molecules, structure modification to increase potency-homologation, chain branching, ring chain transformation, bioisosterism, combinatorial chemistry-general aspects, solid – phase mix and split synthesis, parallel chemical synthesis and encoding techniques. Structure modification to increase oral bioavailability- electronic effects, lipophilicity effects.

1.2 Quantitative structure activity relationships: Steric effects, Hansch analysis, de novo method, Topliss method. Computer–Based Methods of QSAR, Basic concepts of CADD, molecular modeling, molecular docking. Introduction to 2D & 3D QSAR. (18 Hrs)

1.3 Retrosynthetic analysis: Introduction to Retrosynthetic analysis and disconnection approach-synthetic strategy and synthons- Retrosynthetic analysis of benzocaine, saccharin, salbutamol and benzodiazepines. (5 Hrs)

1.4 Receptors: Classification of receptors, Drug- receptor interactions, Theories of Drug-receptor interactions, stereochemical aspects, drug–receptor chirality, geometrical isomers, conformational isomers, ring topology. (4 Hrs)

Module 2: Basic principles of Drug Design and Pharmacology (9 Hrs)

2.1 General principles of pharmacology: Drug nomenclature, orphan drugs, Concept of prodrugs and soft drugs. Routes of drug administration, biological response to drugs.

2.2 Pharmacokinetic principles: Passage of drugs across membranes, absorption, distribution, metabolism-Phase I and Phase II reactions, and excretion of drugs.

2.3 Pharmacodynamic principles: Principles of drug action, mechanism of drug action, dose-response relationships, drug selectivity, unusual and adverse responses of drugs, structurally specific and nonspecific drugs.

2.4 Drug interactions: Synergism, antagonism, drug addiction, drug abuse, drug dependence, drug tolerance, drug hypersensitivity, Immunoglobulins.

Module 3: Inorganic pharmaceutical chemistry (9 Hrs)

3.1 Preparation and uses of the following compounds used in pharmacy: Aluminium hydroxide gel, calcium lactate, calcium gluconate, ferrous fumarate, ferric ammonium citrate, ferrous sulphate, calamine, zinc oxide, zinc stearate, magnesium stearate, talc, yellow mercuric oxide, trivalent and pentavalent antimonials, selenium sulfide, lithium salts, gold, platinum and bismuth compounds,metal complexes used in medicine.

3.2 Metal toxicity - cadmium, lead, copper and mercury.

Study of the chemistry, SAR and uses of the following classes of compounds. Synthesis needed only for the mentioned compounds.

Module 4: Drugs acting on CNS (18 Hrs)

4.1 General anaesthetics: Inhalation anaesthetics - ether, enflurane, halothane, nitrous oxide, cyclopropane. Intravenous anaesthetics–thiopentone sodium, ketamine.

4.2 Hypnotics, sedatives and anxiolytic agents: Barbiturates, benzodiazepines, and miscellaneous- chlordiazepoxide, meprobamate. Anxiolytic agents-benzodiazepines, buspirone, meprobamate.

4.3 Anticonvulsants: Convulsions, types of epilepsy, barbiturates, hydantoins, oxazolidinediones, succinimides, benzodiazepines.

4.4 Analeptics: Xanthines, amphetamines, nikethamide and ethamivan.

4.5 Tranquilisers: Rauwolfia alkaloids, meprobamate, oxazepam, benzodiazepines, chlordiazepoxide, phenothiazene derivatives.

4.6 Antidepressants: MAO inhibitors- Isocarboxazide, tranylcypromine and phenelzine. Tricyclic compounds -imipramine, amitriptyline. Miscellaneous compounds- fluoxetine and trazodone.

4.7 Antipsychotics: Phenothiazine derivatives, thiothixene derivatives, butyrophenone derivatives-haloperidol, rauwolfia alkaloids.

4.8 Hallucinogens: Triptamine derivatives- DMT, psilocybin, phenylalkylamines- mescaline, Lysergic acid derivatives-LSD, Cannabinol compounds.

4.9 Synthesis of the following drugs: Enflurane, Phenobarbital, Chlordiazepoxide, Buspirone, Nikethamide.

Module 5: Analgesics and Antipyretics (9 Hrs)

5.1 Narcotic analgesics: morphine and its analogues, phenyl (ethyl) piperidines, diphenyl heptanones and benzazocin derivatives.

5.2 Antipyretics and NSAIDs: Basic idea of COX I & COX II inhibitors, salicylates- aspirin; p-aminophenol derivatives- paracetamol; pyrazolidinedione derivatives–phenylbutazone, oxyphenbutazone; anthranilic acid derivatives- mefanamic acid, flufenamic acid; indoleacetic acid derivatives- indomethacin; arylacetic/propionic acid derivatives- ibuprofen, and diclofenac; oxicams – piroxicam; selective COX II inhibitors-celecoxib.

5.3 Anti- gout drugs: allopurinol, colchicine.

5.4 Centrally acting muscle relaxants: glyceryl ethers- mephenesin; alkanediol derivatives-meprobamate; benzodiazepines-librium, diazepam; miscellaneous compounds-baclofen.

5.5 Synthesis of the following drugs: Meperidine, phenylbutazone, flufenamic acid, diclofenac, piroxicam and celicoxib.

References

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PG3PHA C12 SPECTROSCOPIC METHODS IN CHEMISTRY

Credit: 3 **Contact Lecture Hours: 54**

Module1: Ultraviolet-Visible and Chiro optical Spectroscopy (9 Hrs)

1.1 Energy levels and selection rules, Woodward-Fieser and Fieser-Kuhn rules.

1.2 Influence of substituent, ring size and strain on spectral characteristics. Solvent effect, Stereochemical effect, non-conjugated interactions.

1.3 Problems based on the above topics.

1.4 Chirooptical properties-ORD, CD, octant rule, axial halo ketone rule, Cotton effect.

Module 2: Infrared Spectroscopy (9 Hrs)

2.1 Fundamental vibrations, characteristic regions of the spectrum (fingerprint and functional group regions), influence of substituent, ring size, hydrogen bonding, vibrational coupling and field effect on frequency, determination of stereochemistry by IR technique.

2.2 IR spectra of C=C bonds (olefins and arenes) and C=O bonds.

2.3 Problems on spectral interpretation with examples.

Module 3: Nuclear Magnetic Resonance Spectroscopy (18 Hrs)

3.1 Magnetic nuclei with special reference to ^{1}H and ^{13}C nuclei. Chemical shift and shielding/deshielding, factors affecting chemical shift, relaxation processes, chemical and magnetic non-equivalence, local diamagnetic shielding and magnetic anisotropy. ^{1}H and ^{13}C NMR scales.

3.2 Spin-spin splitting: AX, AX_2, AX_3, A_2X_3, AB, ABC, AMX type coupling, first order and non-first order spectra, Pascal's triangle, coupling constant, mechanism of coupling, Karplus curve, quadrupole broadening and decoupling, diastereomeric protons, virtual coupling, long range coupling. NOE and cross polarization.

3.3 Simplification of non-first order spectra to first order spectra: shift reagents, spin decoupling and double resonance, off resonance decoupling. Chemical shifts and homonuclear/heteronuclear couplings. Basis of heteronuclear decoupling, ^{19}F and ^{31}P

3.4 2D NMR and COSY, HOMOCOSY and HETEROCOSY

3.5 Polarization transfer, Selective Population Inversion. DEPT. Sensitivity enhancement and spectral editing, MRI.

3.6 Problems on spectral interpretation with examples.

Module 4: Mass Spectrometry (9 Hrs)

4.1 Molecular ion: ion production methods (EI). Soft ionization methods: SIMS, FAB, CA, MALDI, Field Desorption Electrospray Ionization.Magnetic, TOF, quadrupole and ion cyclotron mass analyzers. MS^n technique. Fragmentation patterns- nitrogen and ring rules. McLafferty rearrangement and its applications. HRMS, MS-MS, LC-MS, GC-MS.

4.2 Problems on spectral interpretation with examples.

Module 5: Structural Elucidation Using Spectroscopic Techniques (9 Hrs)

5.1 Identification of structures of unknown organic compounds based on the data from UV-Vis, IR, ^1H NMR and ^{13}C NMR spectroscopy (HRMS data or Molar mass or molecular formula may be given).

5.2 Interpretation of the given UV-Vis, IR and NMR spectra.

References

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11. E.B. Wilson Jr., J.C. Decius, P.C. Cross, Molecular Vibrations: The Theory of Infrared and Raman Vibrational Spectra, Dover Pub., 1980.

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SEMESTER 4

ELECTIVE COURSES

(Any 3 courses to be opted from the following courses)

PG4PHA E01 BACTERIOLOGY AND BIOCHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Introduction to Microbiology (9 Hrs)

1.1 A general study of viruses, fungi and protozoa. Morphology, classification and scientific nomenclature of bacteria. Growth requirements of bacteria. Classification of nutrient media. Applications of nutrient media in the practice of bacteriology. Staining of bacteria, theories of staining. Viral infections, methods of viral multiplication, causing of diseases, bacteriophages. General principles of microbial control- sterilization, disinfection, prions.

1.2 Cells- classification and cell division

Module 2: Immunity (9 Hrs)

Types of immunity. Antigens and antibodies: theories of antigen-antibody reactions, AIDS, applications of antigen-antibody reactions. Interferons. Vaccines and sera - general study of the preparation of different types of vaccines, sera and toxoids. Monoclonal antibodies.

Module 3: Amino acids, Proteins and Nucleic Acids (18 Hrs)

3.1 Amino acids and Proteins: Essential amino acids. Primary structure of proteins and amino acid analysis. Ramachandran plot and secondary structure of proteins. Tertiary structure and structural motifs- protein folding and domain structure of proteins. Quaternary structure of proteins. Purification and characterization of proteins. Functions of proteins. Chemical synthesis of proteins- protecting groups, solution and solid phase peptide synthesis.

3.2 Nucleic acids: DNA and RNA. Double helical structure of DNA. Replication of DNA. Classification of RNA. Genetic code. Nucleic acids as carriers of genetic information. Protein biosynthesis. Transcription, translation, DNA finger printing technique. Elementary principles of

Recombinant DNA technology, gene therapy, cloning and bioinformatics. Human genome project, DNA profiling and Polymerase chain reaction.

Module 4: Enzymes and Hormones (18 Hrs)

4.1 Enzymes: Nomenclature and classification of enzymes. Mechanism of enzyme action. Substrate specificity of enzymes. Enzyme inhibition. Isoenzymes. Allosteric enzymes. Enzyme synthesis. Enzymes and digestion of food. Clinical uses of enzymes. Immobilization of enzymes. Clinical tests for sugar and cholesterol.

4.2 Hormones: Functions and modes of actions of hormones. Pituitary, thyroid, parathyroid, pancreatic, adrenal and adrenocortical hormones. Male and female sex hormones. Antihormones.

Module 5: Metabolism (18 Hrs)

5.1 Carbohydrate metabolism: Glycogenesis and Glycolysis. Blood sugar level. Cori cycle. The role of insulin. The citric acid cycle. Genetic and metabolic disorders. Diabetes mellitus (type 1 and type 2). Lipaemia.

5.2 Lipid metabolism: β-oxidation of fatty acids. Ketogenesis and ketosis. Biosynthesis of fatty acids. Essential fatty acids. Prostaglandins- nomenclature, structure and biosynthesis.

5.3 Metabolism of amino acids and proteins: Oxidative deamination and transamination reactions. Urea formation- ornithine cycle. Inborn errors of metabolism.

Module 6: Biological Oxidation and Electron Transport Chain (9 Hrs)

6.1 Biological Oxidation: High energy compounds, ATP and ADP. Substrate level and oxidative phosphorylation. Electron transport chain, Cytochromes.

6.2 Food as a source of energy. Calorific value of food. Basal metabolism. Respiratory quotient.

Module 7: Blood Composition and Acid Base Balance (9 Hrs)

7.1 Blood groups- Rh factor. Blood transfusion. Composition of blood cells. Chemistry of haemoglobin. Anaemias. Plasma proteins. Blood clotting- factors and mechanism. Coagulants.

7.2 Regulation of acid base balance. Acidosis and alkalosis. Renal function. Formation and composition of urine. Diabetes insipidus.

References

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PG4PHA E02 PHARMACOGNOSY & PHARMACEUTICAL OPERATIONS

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Pharmacognosy-1 (18 Hrs)

Pharmacognosy of the official drugs frequently used in pharmacy: Names, sources, chemical constituents, macroscopial characters and uses of senna, belladona, digitalis, stramonium, vasaka, cinnamon, cinchona, ergot, ipecacuanha, rauwolfia, liquorice, ginger, cloves, pyrethrum, santonica, nutmeg, nuxvomica, cardamom, umbelliferous fruits like Cumin, Fennel, Caraway, Opium, Aloes, Asafoetida, Vinca rosea, Brahmi (two varieties).

Module 2: Pharmacognosy-II (9 Hrs)

2.1 Fixed oils and essential oils used in pharmacy-their sources. Extraction, constituents, composition and analysis of fixed oils. Elementary study of adulteration of fixed oils.

2.2 Fixed Oils: Castor oil, Olive oil, Shark liver oil, cod liver oil.

2.3 Essential Oils: Eucalyptus oil, Turpentine oil. Uses of essential oils in medicine – Aromatherapy.

2.4 A brief study of the substances used as pharmaceutical necessities – Starches, gum acacia, gum tragacanth, agar- agar, gelatin, talc, kaolin, bentonite and white petroleum jelly, wools fat, lanolin, bees wax, yellow bees wax.

Module 3: Dispensing (9 Hrs)

3.1 Principles of dispensing medicaments. Incompatibilities and overcoming of incompatibilities. Preparation of pills, tablets, capsules, injectables, emulsions, suppositories, coating of tablets.

3.2 Newer Drug Delivery systems: Site specific drug delivery systems – to brain, CNS, GIT, kidney and urinary tract and in cancer chemotherapy, controlled release phenomena, slow release phenomena, implanted mechanical pumps.

Module 4: Forensic Pharmacy (18 Hrs)

4.1 Pharmaceutical Legislation in India. Legal aspects of trade in drugs. The drug Act and Drug rules. The Pharmacy Act. The dangerous drug Act and Rules. The Drugs and Cosmetic Act and rules

4.2 Introduction to Pharmacopeia- B.P, I.P. and general standard analysis.

4.3 Intellectual Property Rights (IPR), Patents, Trademarks, Copy rights, Patent Acts relevant sections (basic ideas only).

Module 5: Pharmaceutical Operations (18 Hrs)

5.1 Principles involved, Apparatus and machinery used in general pharmaceutical operations of IP/BP - evaporation, extraction, crystallization, distillation.

5.2 Chromatographic techniques: theory of chromatography, Applications of adsorption, partition, paper, thin layer and column chromatographic methods. LC, HPLC, IEC, GC and GPC. Column matrices. Detectors. Affinity and chiral columns.

5.3 Electrophoresis - general ideas. Ultracentrifugation.

5.4 Solvent extraction, liquid – liquid extraction, uses of oxine, dithiazone, dithiocarbamates, high molecular weight amines and crown ethers in extraction.

Module 6: Nanotechnology and Green Chemistry (9 Hrs)

6.1 Applications of nanomaterials in medicine: immunogold labelling, applications in medical diagnosis, nano based drug delivery, biomimetic nanotechnology, DNA nanotechnology and structural biomimicry.

6.2 Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis.

6.3 Green alternatives of organic synthesis: coenzyme catalyzed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay-catalyzed synthesis, condensation reactions. Green photochemical reactions. Microwave assisted organic synthesis.

6.4 Green chemistry in pharmaceutical industry: Ibuprofen manufacture, bio-catalysis.

Module 7: Polymers and Diagnostic agents (9 Hrs)

7.1 Conducting polymers, Polymers for NLO applications, Polymers for medical applications, Dendrimers- Methods of synthesis, dendrimers as nanocapsules, Applications of dendrimers. Biopolymers and their medical applications.

7.2 Radiopaques – organoiodo compounds. Compounds used in function tests, dyes, radio isotopes, RIA, ELISA, blotting techniques, finger printing studies of DNA.

7.3 Dyes used in pharmacy: fluorescein, mercurochrome, acridine dyes.

7.4 Colouring agents: official colours, colour code.

7.5 Liver and gastric function tests and kidney function tests.

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PG4PHA E03 MEDICINAL CHEMISTRY- II

Credit: 4 **Contact Lecture Hours: 90**

Module1: Drugs acting on ANS (18 Hrs)

1.1 Adrenergic stimulants: α- and β- adrenoreceptor agonists, Phenyl ethanolamine derivatives-adrenaline, isoprenaline, salbutamol, ephedrine, and phenylephrine. Imidazoline derivatives- naphazoline, xylometazoline and oxymetazoline.

1.2 Adrenergic blockers: α- and β- adrenoreceptor antagonists- ergot alkaloids, phenoxybenzamine, tolazoline, propranolol, atenolol, labetolol. Neuron blockers– bretylium and xylocholine.

1.3 Cholinergic stimulants: Nicotinic and muscarinic receptors, acetylcholine and analogues, pilocarpine, bethanechol and carbachol.

1.4 Cholinergic blockers: Tertiary and quaternary antimuscarinics. Antispasmodic drugs- dicyclomine, glycopyrrolate. Antiulcer drugs- pirenzepine. Cycloplegic drugs- tropicamide, homatropine.

1.5 Anticholinesterases: Competitive inhibitors- physostigmine and neostigmine. Non-competitive inhibitors- organophosphorus compounds, Nerve gases, Cholinesterase regenerators- 2 PAM.

1.6 Antiparkinson's agents: Dopamine agonists, dopamine releasing agents and synthetic anticholinergics. Drugs for Alzheimer's disease: Cholinergic agonists and acetylcholinesterase inhibitors.

1.7 Curare form drugs: Curare alkaloids, erythrina alkaloids and gallamine.

1.8 Synthesis of the following drugs: Salbutamol, carbachol, tolazoline, propranolol.

Module 2: Drugs acting on CVS (18Hrs)

2.1 Cardiotonic drugs: Cardiac glycosides-their chemistry and stereochemistry, Digoxin and digitoxin.

2.2 Antiarrhythmic drugs: Classification, quinidine, disopyramide, lidocaine, phenytoin and procainamide, β-blockers-propranolol. Calcium channel blockers- verapamil and neuron blockers-bretylium.

2.3 Antihypertensive drugs: Classification, Peripheral antiadrenergics- prazosin and terazosin. Centrally acting drugs- reserpine, clonidine and methyl dopa. β-blockers-propranolol, atenolol and labetalol. Direct vasodilators- hydralazine and minoxidil. Ganglion blocking agents-mecamylamine and trimethophan. Calcium channel blockers- nifedipine and amlodipine. ACE inhibitors- captopril. Angiotensin receptor blockers- losartan. Diuretics- thiazide diuretics.

2.4 Antianginal drugs: Vasodilators- nitrites and nitrates, β-blockers- propranolol, atenolol, nadolol. Calcium channel blockers- verapamil and nifedipine. Miscellaneous- dipyridamole and aspirin.

2.5 Anticoagulants: Heparin, coumarin derivatives and indanedione derivatives.

2.6 Hypolipidaemic agents: Atherosclerosis (elementary idea only), Statins-lovastatin, fluvastatin, atorvastatin. Fibrates- clofibrate. Miscellaneous- bile acid sequestrants and cholestyramine resin and Gugulipid.

2.7 Synthesis of the following drugs: Disopyramide, amlodipine, verapamil, captopril and fluvastatin.

Module 3: Chemotherapy (18 Hrs)

3.1 Antibiotics: β-lactam antibiotics- penicillins and cephalosporins, natural, biosynthetic and semisynthetic penicillins, tetracyclines and chloramphenicol, A brief study of macrolide antibiotics, aminoglycoside antibiotics and polyene antibiotics. Fluoroquinolones.

3.2 Sulphonamides: Sulphanilamide, N-substituted sulphanilamide derivatives, mechanism of action, sulphones- dapsone, dihydrofolate reductase inhibitors-trimethoprim and cotrimoxazole.

3.3 Antimicobacterial agents: A brief study of infection, its development and social significance. Antitubercular agents: first line drugs- isoniazid, rifampicin, pyrazinamide, ethambutol, and streptomycin. Second line drugs- ethionamide, para aminosalicylic acid, kanamycin and fluoroquinolones. Types of leprosy, Antileprotic drugs- dapsone, phenazine derivatives-clofazimine.

3.4 Antifungal agents: Systemic and topical antifungal agents- Antibiotics-amphotericin B, griseofulvin and nystatin. Azole derivatives- ketoconozole, fluconozole and clotrimazole. Pyrimidine derivatives- 5- Flucytosine.

3.5 Antiviral drugs: A brief study of infection, its development and social significance. Principles of antiviral drugs. Nucleoside and non-nucleoside analogues. Anti-herpes virus drugs- Idoxuridine, vidarabine and acyclovir. Anti-retro virus drugs- zidovudine and abacavir. Anti-influenza virus drugs- amantadine, oseltamivir (tamiflu). Nonselective antiviral drugs- interferons and ribavirin.

3.6 Antiprotozoal agents: A brief study of infection, its development and social significance. Amoebicides: Ipecacuanha alkaloids- emetine, dehydroemetine, metranidazole and tinidazole. Antimalarials: Life cycle of parasite. 4-aminoquinolines, 8-amino quinolines, acridine and artemesinine derivatives. Anthelmintics: piperazines and benzimidazoles. Taeniasis- albendazole.

3.7 Synthesis of the following drugs: Ampicillin, cephalexin, chloramphenicol, sulphamethoxazole, dapsone, metronidazole.

Module 4: Antineoplastic Drugs (9 Hrs)

4.1 Neoplasm: cause, therapeutic approaches. Classification of drugs, Alkylating agents- nitrogen mustards, nitrosourea, aziridines and aryl sulphonates. Antimetabolites- folic acid antagonists, purine and pyrimidine antagonists. Antibiotics- anthracyclines, actinomycin D and bleomycin. Plant products- vinca alkaloids, taxol derivatives. Hormones and their antagonists- tamoxifen. Miscellaneous- procarbazine, cisplatin.

4.2 Synthesis of the following drugs: chlorambucil, thiotepa, methotrexate, 5-fluoro uracil.

Module 5: Antihistaminic drugs and Gastrointestinal drugs (9Hrs)

5.1 Antihistaminic drugs: Histamine and its biological role, H_1 receptor antagonists-aminoalkyl ethers- diphenhydramine and doxylamine. Ethylenediamine derivatives-pyrilamine, phenothiazines- promethazine, trimeprazine, piperazine derivatives- cyclizine, miscellaneous compounds- cetrizine and cyproheptadine.

5.2 Drugs for peptic ulcer: Antacids- systemic and non- systemic antacids, H_2 receptor antagonists- cimetidine, ranitidine and famotidine. Proton pump inhibitors- omeprazole and pantoprazole. Anti-H.pylori drugs, Gastroesophageal reflux disease (GERD).

5.3 Purgatives: Irritant, osmotic, bulk and lubricant purgatives, digestants, carminatives and antidiarrhoeals.

5.3 Synthesis of the following drugs: Diphenhydramine, pyrilamine, promethazine, omeprazole.

Module 6: Miscellaneous class of compounds (18 Hrs)

6.1 Diuretics: Common diuretics and their mechanism of action. Mercurial and non-mercurial diuretics- carbonic anhydrase inhibitors- acetazolamide and methazolamide. Thiazide derivatives- hydrochlorothiazide, Sulphonamides, osmotic diuretics- mannitol, isosorbide, glycerol. Loop diuretics- furosemide and ethacrynic acid, potassium sparing diuretics- amiloride, spironolactone. Antidiuretics- antidiuretic hormone.

6.2 Oral hypogycemic agents: Type 1 and Type 2 diabetes, insulin, suphonylureas-tolbutamide, acetohexamide and glibenclamide, glipizide. biguanides-metformin, thiazolidinediones- rosiglitazone.

6.3 Local anaesthetics: Clinical application of local anaesthesia, coca and cocaine, hexylcaine, para amino benzoic acid derivatives- benzocaine, procaine, tetracaine, anilides, lidocaine.

6.4 Expectorants and Antitussives: Centrally acting antitussives- opium alkaloids and synthetic substitutes- codeine, noscapine, pholcodine, ethyl morphine, dextromethorphan. Expectorants- terpin hydrate, guaicol and bromhexine.

6.5 Synthesis of the following drugs: Acetazolamide, furosemide, ethacrynic acid, benzocaine, dextromethorphan.

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PG4PHA E04 - POLYMER CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Introduction to Polymer Science (9 Hrs)

1.1 History of macromolecular science: monomers, functionality, degree of polymerization, classification of polymers based on origin, structure, backbone, branching, action of heat, ultimate form and use, tacticity and crystalline behaviour.

1.2 Primary bonds-molecular forces in polymers: dipole forces, induction forces, dispersion forces and H bond, dependence of physical properties on intermolecular forces. Polymer molecular weight-different averages, polydispersity index, molecular weight distribution curve, polymer fractionation. Methods for molecular weight determination: end group analysis, colligative property measurements, ultracentrifugation, vapour phase osmometry, viscometry, GPC, light scattering method. Monomers and structure of common polymers like PE, PP, PVC, PVAc, PVA, PMMA, PEMA, poly lactic acid, PET, PBT, PS, PTFE, PEI, nylon 6, nylon 66, nylon 612, Kevlar, PEEK, PES, PC, ABS, PAN, PEO, PPO, PEG, SAN, PCL, PLA, PHB, DGEBA, MF, UF, AF, PF, PU, NR, SBR, NBR, PB, butyl rubber, polychloroprene and thiokol rubber.

Module 2: Fundamentals of Polymerization (18 Hrs)

2.1 Addition polymerization, free radical addition polymerization, mechanism and kinetics of vinyl polymerization, kinetics of free radical addition polymerization, effect of temperature, pressure, enthalpies, entropies, free energies and activation energies on polymerization.

2.2 Ionic polymerization, common features of two types of ionic polymerization, mechanism and kinetics of cationic polymerization, expressions for overall rate of polymerization and the number average degree of polymerization, mechanism and kinetics of anionic polymerization, expressions for overall rate of polymerization and the average degree of polymerization, living polymers.

2.3 Mechanism of coordination polymerization, Ziegler-Natta polymerization, ring opening polymerization, mechanism of polymerization of cyclic amides.

2.4 Copolymerization, types of copolymers, the copolymer composition equation, reactivity ratio and copolymer structure-influence of structural effects on monomer reactivity ratios, the Q-e scheme, synthesis of alternating, block and graft copolymers.

2.5 Step reaction (condensation) polymerization, Carothers equation, mechanism of step reaction polymerization, kinetics of step reaction polymerization, number distribution and weight distribution functions, polyfunctional step reaction polymerization, prediction of gel point.

2.6 Controlled polymerization methods, nitroxide mediated polymerization, Ring Opening polymerization (ROP), Atom Transfer Radical Polymerization (ATRP), Reversible Addition Fragmentation Termination (RAFT).

Module 3: Properties of Polymers (18 Hrs)

3.1 Structure property relationship in polymers, transitions in polymers, first order and second order transitions in polymers, relationship between Tg and Tm, molecular motion and transitions, Boyer-Beamem rule, factors affecting glass transition temperature.

3.2 Rheological properties of polymers, Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venant body, dialatant, complex rheological fluids, rheopectic fluids, time dependent fluids, time independent fluids, power law, Weissenberg effect, laminar flow, turbulent flow, die swell, shark skin, viscous flow.

3.3 Viscoelastic properties of polymers, viscoelasticity, Hooke's law, Newton's equation, viscoelastic models-time temperature equivalence, WLF equation, Boltzmann superposition principle, linear stress - strain relations for other types of deformation-creep, stress relaxation. Temperature dependence of viscosity. Transport in polymers - diffusion, liquid and gas transport, Fick's law, theories of diffusion.

Module 4: Stereochemistry and Conformation of Polymers (9 Hrs)

Stereoregular polymers, constitutional isomerism, positional isomerism and branching, optical isomerism, geometric isomerism, substitutional isomerism, configuration of polymer chains, infrared, Raman and NMR characterization, polymer conformation, chain end to end distance, random walks and random flights, self-avoiding walks.

Module 5: Morphology and Order in Crystalline Polymers (9 Hrs)

5.1 Polymer morphology, common polymer morphologies, structural requirements for crystallinity, degree of crystallinity, crystallisability- mechanism of crystallization, polymer single crystals, lamellar structure of polymers, fringed micelle concept, folded chain model, adjacent re-entry model, switchboard model.

5.2 Structure of polymers crystallised from melt, spherulitic morphology, mechanism of spherulite formation, theories of crystallisation kinetics, Avrami equation, Hoffman's nucleation theory, the entropic barrier theory, strain induced morphology, cold drawing, morphology changes during orientation, application of XRD, SEM and DSC in determining the crystallinity of polymers.

Module 6: Advances in Polymers (9 Hrs)

6.1 Specialty polymers, conducting polymers, high temperature polymers, flame resistant polymers, biopolymers and biomaterials, polymers in medicine, polymers for dental applications

6.2 Carbon fibres. Synthesis, characterization and applications of carbon nanofibres.

Module 7: Dendrimers and Dendritic Polymers (18 Hrs)

7.1 Basic concepts and terminology: Dendrons, star shaped and starbust polymers, dendrimer formation and generations, various types of dendrimers.

7.2 Synthesis of dendrimers-convergent and divergent approaches, methods and mechanism. Properties of dendrimers- polydispersity, mechanical properties, viscoelastic properties. Determination of physical properties.

7.3 Characterisation of dendrimers: GPC, osmosis, TG, DSC, magnetic resonance spectroscopy (proton and carbon-13 NMR), mass spectral studies (MALDI and TOF).

7.4 Dendritic macromolecules: hypergrafted and hyperbranched polymers - definition and classification, synthesis-methods and mechanism, characterization, properties, applications.

References

[1] V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age International, 2003.

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PG4PHA E05 ANALYTICAL CHEMISTRY

Credit: 4 **Contact Lecture Hours: 90**

Module 1: Instrumental Methods (36 Hrs)

1.1 Electrical and nonelectrical data domains-transducers and sensors, detectors, examples for piezoelectric, pyroelectric, photoelectric, pneumatic and thermal transducers. Criteria for selecting instrumental methods-precision, sensitivity, selectivity, and detection limits.

1.2 Signals and noise: sources of noise, S/N ratio, methods of enhancing S/N ratio hardware and software methods.

1.3 Electronics: transistors, FET, MOSFET, ICs, OPAMs. Application of OPAM in amplification and measurement of transducer signals.

1.4 UV-Vis spectroscopic instrumentation: types of optical instruments, components of optical instruments-sources, monochromators, detectors. Sample preparations. Instrumental noises. Applications in qualitative and quantitative analysis.

1.5 Molecular fluorescence and fluorometers: photoluminiscence and concentration electron transition in photoluminescence, factors affecting fluorescence, instrumentation details. Fluorometric standards and reagents.Introduction to photoacoustic spectroscopy.

1.6 IR spectrometry: instrumentation designs-various types of sources, monochromators, sample cell considerations, different methods of sample preparations, detectors of IR-NDIR instruments. FTIR instruments. Mid IR absorption spectrometry. Determination of path length. Application in qualitative and quantitative analysis.

1.7 Raman Spectrometric Instrumentation: sources, sample illumination systems. Application of Raman Spectroscopy in inorganic, organic, biological and quantitative analysis.

1.8 NMR Spectrometry-magnets, shim coils, sample spinning, sample probes (1H, 13C, 32P). Principle of MRI.

Module 2: Sampling (18 hrs)

2.1 The basis and procedure of sampling, sampling statistics, sampling and the physical state, crushing and grinding, the gross sampling, size of the gross sample, sampling liquids, gas and

solids (metals and alloys), preparation of a laboratory sample, moisture in samples-essential and non essential water, absorbed and occluded water, determination of water (direct and indirect methods).

2.2 Decomposition and dissolution, source of error, reagents for decomposition and dissolution like HCl, H_2SO_4, HNO_3, $HClO_4$, HF, microwave decompositions, combustion methods, use of fluxes like Na_2CO_3, Na_2O_2, KNO_3, NaOH, $K_2S_2O_7$, B_2O_3 and lithium metaborate. Elimination of interference from samples-separation by precipitation, electrolytic precipitation, extraction and ion exchange.Distribution ratio and completeness of multiple extractions.Types of extraction procedures.

Module 3: Applied Analysis (9 hrs)

3.1 Analytical procedures involved in environmental monitoring. Water quality- BOD, COD, DO, nitrite, nitrate, iron, fluoride.

3.2 Soil-moisture, salinity, colloids, cation and anion exchange capacity.

3.3 Air pollution monitoring sampling, collection of air pollutants-SO_2, NO_2, NH_3, O_3 and SPM.

3.4 Analysis of metals, alloys and minerals. Analysis of brass and steel. Analysis of limestone. Corrosion analysis.

Module 4: Capillary Electrophoresis and Capillary Electro Chromatography (9 Hrs)

4.1 Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection (indirect)-fluorescence, absorbance, electrochemical, mass spectrometric, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.

4.2 Capillary electro chromatography- packed columns. Micellar electro kinetic chromatography.

Module 5: Process instrumentation (9 Hrs)

Automatic and automated systems, flow injection systems, special requirements of process instruments, sampling problems, typical examples of C, H and N analysers.

Module 6: Aquatic Resources (9 Hrs)

6.1 Aquatic resources: renewable and non-renewable resources, estimation, primary productivity and factors affecting it, regional variations.

6.2 Desalination: principles and applications of desalination-distillation, solar evaporation, freezing, electrodialysis, reverse osmosis, ion exchange and hydrate formation methods. Relative advantages and limitations. Scale formation and its prevention in distillation process.

6.3 Non-renewable resources: inorganic chemicals from the sea-extraction and recovery of chemicals, salt from solar evaporation.

References

[1] J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.

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[5] G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.

[6] J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.

[7] J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.

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SEMESTERS 3 & 4

PG4PHA P04: PHARMACEUTICAL ANALYSIS & PHARMACOGNOSY PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I

Preparation, assay including limit tests prescribed in the IP/BP of the following drugs: sodium salicylate, calcium lactate, yellow mercuric oxide, ferrous fumarate, ferric ammonium citrate.

PART II

1. Assay of the following synthetic drugs: 1. Aspirin, 2. Paracetamol, 3. Sulphadiazine (or any other sulphonamide), 4. Isoniazid, 5. Benzyl benzoate, 6. Oxyphenbutazone.
2. Determination of Iodine value and Saponification value of fixed oil (Olive oil)
3. Colorimetric/Spectrophotometric determination of 1) Aniline 2) Glucose 3) Cholesterol 4) Ascorbic acid 5) Streptomycin, 6) Aspirin, 7) sulpha drug (Sulphadiazine, Sulphaguanidine).
4. Analysis of official drugs using common analytical techniques- Amperometric analysis of sulpha drugs
5. Assay of Vitamins: ascorbic acid, niacinamide, pyridoxine and thiamine.
6. Assay of some alkaloids official in IP/BP: atropine, codeine, ephedrine and quinine. Analysis of liquid extracts of some alkaloidal content.

PART III

Macroscopic examination, identification, description with constituents present and pharmacological action of crude drugs (15 common medicinal plants are to be studied).

PART IV- Viva voce

References

[1] A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.

[2] G.L. Genkins, A.M. Knevel, F.E. DiGangi, Quantitative Pharmaceutical Chemistry, 7th Edn., McGraw Hill, 1977.

[3] K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.

[4] Indian Ministry of Health and Family Welfare, Indian Pharmacopoeia 1996, Controller of Publication, 2000.

[5] British Pharmacopoeia Commission, British Pharmacopoeia: 2012 Edition, Bernan Assoc., 2011

[6] M.A. Iyengar, Pharmacognosy of Crude Drugs.

[7] T.E.Wallis, Practical Pharmacognosy, Churchill, London, 1955.

PG4PHA P05 DRUG SYNTHESIS AND DISPENSING PRACTICAL

Credit: 3 **Contact Lab Hours: 54+54=108**

PART I Preparation of drug and drug intermediates.

I. Preparation Involving Multistep Synthetic Sequences

1. Benzaldehyde –Benzoin-benzyl.
2. Benzoin--Benzil-Dilantin
3. Phthalic acid-- Phthalic anhydride—phthalimide-- anthranilic acid
4. Flourescein---Dibromofluorescein---Mercurochrome
5. Methyl benzoate –methyl m-nitrobenzoate—m-nitrobenzoic acid
6. Aniline—acetanilide—p-nitroacetanilide
7. Acetanilide- 4-Acetamidobenzene sulphonyl chloride-4-Acetamido benzenesulfonamide-- Sulphanilamide

II. Preparation Involving Green Alternatives of Chemical Methods

1. Bisnaphthol from 2-naphthol
2. Coenzyme catalyzed benzoin condensation using thiamine hydrochloride
3. Photoreduction of benzophenone to benzopinacol using isopropanol
4. Benzopinacol to benzopinacolone
5. Acetanilide from aniline using zinc dust

III. Microwave assisted Organic Synthesis

1. 2-Hydroxychalcone from salicylaldehyde and acetophenone
2. 3-Methyl-1-phenyl-5-pyrazolone from ethyl acetoacetate
3. Benzoic acid from ethyl benzoate
4. Ethyl- 3-nitrobenzoate from 3- nitrobenzoic acid

PART II

Prediction of FTIR, ^{1}H and ^{13}C NMR spectra of the intermediates and products at each stage of synthesis by the above methods.

PART III Dispensing

1.Emulsions: a. Castor oil emulsion, b. Shark liver oil emulsion, c. Liquid paraffin emulsion

2.Liniments: a. Turpentine liniment, b. Methyl salicylate liniment c. Camphor liniment

3.Mixtures: Typical mixtures involving incompatibilities.

PART IV- Viva voce

References

[1] A.I. Vogel, A Textbook of Practical Organic Chemistry, Longman, 1974.

[2] A.I. Vogel, Elementary Practical Organic Chemistry, Longman, 1958.

[3] F.G. Mann and B.C Saunders, Practical Organic Chemistry, 4th Edn., Pearson Education India, 2009.

[4] J.R. Adams, J.R. Johnson, J.F. Wilcox, Laboratory Experiments in Organic Chemistry, Macmillan, 1979.

[5] V.K. Ahluwalia, Green Chemistry: Environmentally Benign Reactions, Ane Books, 2009.

[6] Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST, 2009.

[7] R.M Silverstein, Spectrometric Identification of Organic compounds.

[8] F. G. Mann and B.C. Saunders, Practical Organic Chemistry, Pearson.

[9] J. B. Cohen, Practical Organic Chemistry, Mc Graw Hill.

[10] C.E Bella and DF Taber, Organic Chemistry Laboratory, Thomson.

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[12] A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.

[13] K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.

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PG4PHA P06 BIOCHEMISTRY AND BACTERIOLOGY PRACTICAL

Credit: 3 **Contact Lab Hours: 72+72 =144**

Biochemistry

PART I

1. Blood Analysis

a. Determination of blood group and Rh factor, b. Enumeration of RBC, WBC and differential leucocyte count, c. Determination of ESR, d. Estimation of urea, uric acid, cholesterol, creatinine, haemoglobin and calcium.

2. Urine Analysis

a. Qualitative analysis of urine for the common pathological constituents-sugar, albumin, ketone bodies, bile, b. Estimation of albumin, ketone bodies, sugar and urea

3. Milk Analysis

Estimation of specific gravity, total solids, fat, lactose, total nitrogen, calculation of percentage of added water.

4. Water Analysis

Sample collection, Fixing of DO, Determination of refractive index, salinity, DO, BOD, COD, nitrite, sulphate, nitrate, phosphate, silicate analysis, Microbial analysis. Estimation of total dissolved matter, chloride, saline and albuminoid ammonia and COD.

PART II

1. Isolation of phytochemicals from their natural sources.

   1) Caffeine from Tea, 2) Nicotine from tobacco, 3) Curcumin from turmeric, 4) Tannins from Gallnuts 5) Lycopene from tomato.

2. Separations of mixtures by Paper Chromatography- 1) Separation of amino acids 2) Separation of dyes
3. Separation of serum proteins by paper electrophoresis.

Bacteriology

PART III

1) Preparation of some typical nutrient media for collection and isolation of bacteria.
2) Nutrient Agar, Endo's Agar, Chapman's Agar, Tergotol-7 Agar and McConkey Agar.
3) Staining and the study of the morphology of the bacteria.
4) Simple stain, b. Gram stain (Huker method), c. Negative stain (India ink method)
5) Fermentation test
6) Identification of some common pathogenic organisms.
7) Method of study of antibacterial activity of compounds and complexes.

PART IV- Viva voce

References

[1] A.J. Salle, Laboratory Manual of Fundamental Principles of Bacteriology, McGraw Hill, 1973.

[2] R.C. Goss, Experimental Microbiology Laboratory Guide, Iowa State Univ. Press, 1967.

[3] T.J. Mackie, J.E. McCartney, Handbook of Practical Bacteriology, E & S Livingstone, 1948.

[4] P.B. Hawk, Hawk's Physiological Chemistry, Blakiston Division, 1965.

[5] K. Wilson and J.M. Walker, Principles and Techniques of Practical Biochemistry, 5th Edn., Cambridge University Press, 2000.

[6] M.B. Jacob, The Chemical Analysis of Food and Food products, Van Nostrand, 1958.

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M.Sc. Degree Pharmaceutical Chemistry Programme

Aim and Objective of the Syllabi
Outcome

The curriculum provides valuable knowledge of various subjects like biochemistry, medicinal chemistry, pharmacognosy, pharmacology etc.A candidate can pursue a Master's Degree in Pharmaceutical Chemistry which offers various specializations like biochemistry, medicinal chemistry, pharmacognosy, pharmacology etc.After obtaining the Master's Degree and then for further research work can go for it.

Aim
Chemistry is a central subject of science. It is also closely related to daily life. The Master's program not only offers the option of focusing on a specialist area but students will also acquire the necessary skills for this and they will learn to think independently and act responsibly.Graduates will become familiar with the terminologies and special aspects of chemistry, its strengths and limitations and will be able to apply their knowledge to new issues and situations, even in an interdisciplinary context. They will gain knowledge and practical skills relating to the current state of research in selected fields. They will be able to analyze chemical issues and assess them critically, to develop independent solution strategies and to estimate their impacts in a wider context. The broad spectrum of the academic program will ensure that students acquire the skills necessary for demanding fields of activity in industry, economy and administration

Objective
The Master's course in chemistry is designed with an objective to teach post graduates with the skills to critically assess and deal with issues requiring the utilization of chemical principles from each sub-disciplines such as organic, inorganic, physical, analytical and biochemistry. It is the objective of the chemistry program to teach students the necessary knowledge in a way that enables them to familiarize themselves quickly with new developments, to be introduced to new areas and to make independent contributions to further developments of research and technology in their specialized area once they have finished their program.

Semester 1

PG1PHA C01 Inorganic Chemistry - I
Aimand Objectives
This is a chemistry module designed for chemistry majors and features the principles of coordination chemistry, boron compounds and that of nuclear chemistry. In depth discussion about coordination compounds focusing primarily on their structure and various aspects of bonding will be done. The course covers synthesis, structure and bonding of organometallic compounds. Kinetics of reactions of metal complexes and their mechanism will also be illustrated. The learners should be able to apply these topics in various fields.

- To mould the chemistry majors in coordination chemistry, boron compounds and nuclear chemistry
- To understand the structure and various aspects of bondingin the coordination compounds
- To achieve knowledge about the synthesis, structure and bonding of organometallic compounds
- To illustrate the kinetics of reactions and their mechanism of metal complexes
- To acquire ability to apply the theoretical knowledge in various fields

PG1 PHA C02 Organic Chemistry - I

Aim and Objectives

The module deals primarily with the basic principles to understand the structure and reactivity of organic molecules. Emphasis is on substitution and elimination reactions of aliphatic and aromatic compounds. Learners will get the essential ideas on how simple molecules can be constructed. Bonding in conjugated systems, reactions mechanism, organic transformations and stereochemistry will likewise be discussed.

- To understand the structure and reactivity of organic molecules
- To emphasizethe substitution and elimination reactions of aliphatic and aromatic compounds
- To get an idea about the construction of simple organic molecules
- To impart knowledge about stereochemistry of organic compounds and basic principles of conformational analysis
- To know the bonding in conjugated systems and various reaction mechanisms

PG1 PHA C03 Theoretical Chemistry - I

Aim and Objectives

This module looks at quantum chemistry and group theory. A more profound comprehension of quantum chemistry beginning from its postulates and basic systems such as particle-in-a-box to hydrogen like atoms is explored. The second part of the module looks at molecular symmetry and applications in molecular orbitals analysis and vibrational spectroscopy, electronic transitions of carbonyl chromophore and origin of selection rule of electronic transition. Learners will be able to apply these ideas to individual atoms and molecular systems.

- To get a comprehensive idea about quantum chemistry and group theory
- To discuss the emergence of classical mechanics over quantum mechanics
- To get an awareness about the basic postulates of quantum chemistry and its application to hydrogen and hydrogen like atoms
- To acquire knowledge for deriving the wave function, energy, momentum etc. of a particle under different conditions of motions
- To impart knowledge about the molecular symmetry and its applications in molecular orbitals analysis
- To gain information about various spectroscopic techniques, their selection rules and applications based on group theory.
- To solve the problems based on the theories

PG1 PHA C04 Physical Chemistry - I

Aims and Objectives

Physical chemistry is the study of phenomena in chemical systems in terms of physical concepts and laws. In this module, different branches of thermodynamics will be explored. In *ClassicalThermodynamics* kinetic theory of gases, and the energetics of chemical reactions will be explored. Thermodynamics of natural processes and energy transformations in living organisms will be discussed in *Irreversible thermodynamics*. *Statistical Thermodynamics* looks at the relationship between molecular and bulk properties of matter, including examples such as the use of partition functions in equilibrium, transition states and heat capacity of chemical systems. Learners will be familiarized with the behavior of matter in bulk.

- To the study of phenomena in chemical systems in terms of physical concepts and laws

- To analyzedifferent branches of thermodynamics like *ClassicalThermodynamics, Irreversible thermodynamics* and *Statistical Thermodynamics*
- To explore the kinetic theory of gases and the energetics of chemical reactions
- To discuss thermodynamics of natural processes and energy transformations in living organisms
- To correlate themolecular and bulk properties of matter, including partitionfunctions in equilibrium, transition states and heat capacity of chemical systems
- To familiarise the behaviour of matter in bulk
- To solve the problems based on the theories

Semester 2

PG2 PHA C05 Inorganic Chemistry - II
Aim and Objectives
This module coversthree parts: non-aqueous solvents, bioinorganic chemistry and organometallic chemistry. Part 1 deals with acid-base concept and reactions in non-aqueous solvents.Part 2 describes basic principles and concepts of bioinorganic chemistry including the mechanisms of reactions catalyzed by metalloproteins, and kinetics of electron transfer in proteins. Part 3 focusses on thespectral and magnetic properties of transition metal complexes. A comprehensive discussion on inorganic cages and metal clusters follows. The learners will understand the different modes of reactions oforganometallic compounds and their applications can be explored.

- To understand the basic concepts and principles of bioinorganic chemistry
- To familiarise the mechanisms and kinetics of different reactions catalysed by metalloenzymes
- To explore the electronic spectra and magnetic properties of transition metal complexes
- To study the stereochemistry of coordination compounds
- To understand the different reactions and catalysis of organometallic compounds

PG2 PHA C06 Organic Chemistry - II
Aim and Objectives
This module covers the study of a selected series of organic reactions involving reactive intermediates and/or molecular rearrangements. Emphasis is placed on an understanding of their reaction mechanisms. These will include reactions involving carbocations, carbanions, carbenes, carbenoids, nitrenes and arynes as intermediates. Reactions initiated by radicals will be covered. Comprehensive discussions on organic photochemistry including the rules and stereochemical consequences in pericyclic reactions will be given. The learners should be able to apply these ideas in the field of organic synthesis.

- To understand the basic concepts of selected series of organic reactions involving reactive intermediates and/or molecular rearrangements
- To acquire knowledge about name reactions involving radical intermediates
- To understand the symmetry properties of molecular orbitals of selected compounds
- To develop idea about pericyclic reactions
- To understand the basic principles of photochemistry and to apply these principles in different photochemical reactions

PG2 PHA C07 Theoretical Chemistry - II
Aims and Objectives
The objective of this model is to familiarize the learner with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding. Molecular structure evaluation

using group theory will enable the learners to apply it in the field of spectroscopy. To apply the concept of molecular modelling to isolated molecular systems.

- To get idea about various approximation methods to solve many electron systems other than simple systems.
- To discuss the applications of variation method and perturbation method for He atom
- To get an awareness about the SCF, HFSCF methods etc.
- To acquire ability to solve Schrödinger equations for molecules.
- To familiarize with the approximation methods of quantum mechanics and its applications to the various theories of chemical bonding.
- To acquire ability to apply MO treatment to homo and heteronuclear molecules
- To impart knowledge about the HMO theory and its applications to various molecules
- To evaluate molecular structure by using group theory
- To gain information about computational chemistry as a tool and find its applications
- To familiarize different molecular mechanics methods and to understand different force fields
- To achieve knowledge about different methods like HF, Ab initio, molecular mechanics semiempirical, DFT etc.
- To acquire ability to write the Z matrix of different type of molecules
- To familiarize about GAMESS/Firefly and its applications
- To solve the problems based on the theories

PG2 PHA C08 Physical Chemistry - II
Aims and Objectives

In this module, the basic idea of how light interacts with matter, in particular atoms and molecules will be conferred. Microwave, infrared, Raman, electronic and nuclear magnetic resonance spectroscopic techniques will be discussed. Students will be able to apply these principles in the area of molecular spectroscopy.

- To understand the origin of different spectra and characterise the regions of the electromagnetic spectrum.
- To familiarise the microwave spectroscopy and its applications
- To identify Morse potential energy diagram and different types of bands and different types of vibrations and the application of IR spectroscopy
- To get aware about FT spectroscopy and FTIR
- To characterize term symbols and electronic spectra of different molecules
- To identify different types of lasers and realise its applications
- To understand the Mossbauer spectroscopy by learning the principle and recording of spectrum including Doppler effect, chemical shift etc.
- To familiarise the Raman spectroscopy and its applications
- To interpret the complementarities of Raman and IR spectra
- To understand the basic principles of NMR spectroscopy
- To familiarise the second order effects on spectra
- To understand NOE effect, two dimensional NMR, COSY and HETCOR, ^{13}C NMR,
- To familiarise EPR and NQR spectroscopy

PG2 PHA P01 Inorganic Chemistry Practical - I
Aim and Objectives

This is a module intended for chemistry majors. It deals with qualitative and quantitative inorganic analysis along with preparation and characterization of inorganic complexes. The learners will have the option to apply these ideas in various fields pertaining to inorganic chemistry.

- To familiarise different metal salts including rare earths
- To analyse quantitatively different ions using colorimetry
- To characterize the synthesised inorganic complexes

PG2 PHA P02 Organic Chemistry Practical - I
Aim and Objectives
In thismodule,students will learn to apply various techniques to separate a mixture into its individual components and identify each component. Guided under the general principles of analytical and physical chemistry, these techniques include solvent extraction, TLC and column chromatography. Students will also acquire the skill to use the computational tools to draw the reaction schemes and mechanisms of various organic reactions.

- To develop skill in separating different organic mixtures and analyse it
- To familiarise various separation techniques such as solvent extraction, TLC and column chromatography
- To acquire skill to draw structure of organic compounds and the reaction schemes and mechanism of organic reactions using Chemsketch

PG2 PHA P03 Physical Chemistry Practical - I
Aims and Objectives
In this module, students will learn about the practical applications of variousprinciples of physical chemistry like phase rule, adsorption, and surface tension.Learners will be able to use computational software to predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy, and predict its spectral behavior.

- To familiarise different isotherms and to determine the concentration of the given acid using the isotherms
- To construct the phase diagrams of simple eutectics and three component systems
- To acquire knowledge about the effect of salts on miscibility temperature
- To calculate distribution coefficient and equilibrium constant based on distribution law
- To determine the surface tension of a liquid by various methods
- To acquire knowledge about computational software like GAMESS/Firefly
- To predict the geometry of a molecule, calculate its energy levels, assess the HOMO and LUMO energy by using GAMESS/Firefly.

Semester 3

PG3PHA C09 Organic Chemistry- III (Synthetic and Bioorganic Chemistry)
Aims and Objectives

- To enable the students to acquire proper knowledge about various methods of oxidation and reduction reagents. Students will learn about synthetically useful transformations including oxidations and reductions reactions. The emphasis will be on developing a mechanistic understanding of selectivity and synthetic strategy.

- Enable to use various reagents and organic reactions in a logical manner in organic synthesis. An ability to apply synthetic reagents like, DDQ, NBS, DCC, Gilmann reagent etc in organic synthesis and to get insights into novel reactions and reagents in organic synthesis. ·
- To study the important stereoselective transformations in organic synthesis like Asymmetric induction, Enantioselective catalytic hydrogenation, Asymmetric aldol condensation, Asymmetric Diels-Alder reactions and Asymmetric epoxidation.
- The students will be able to understand different approached toward the synthesis of carbocyclic and heterocyclic ring formation etc.
- To impart the students in depth knowledge about the heterocyclic compounds for different elements containing heterocyclic ring and to develop quantitative ideas about the synthesis, properties and uses of such heterocyclic compounds like thiazole, oxazole, pyrimidines, purines, quinoline and isoquinoline.
- To impart the students in depth knowledge about name reactions in cyclisation and construction of macrocyclic rings-ring closing metathesis.
- To get a brief idea and appreciation of the significance and application of supramolecular chemistry and its applications in organic chemistry, chemical biology, medical and perfumery industries. Based on the analysis of a series of host molecules, students able to identify and hypothesize the trends in reactivity and binding of guests.
- To impart the students thorough idea in in the chemistry of terpenoids, steroids, alkaloids and vitamins, proteins and nucleic acids.
- To study the fundamentals of natural colouring species and basic principles of the biosynthesis of terpenes, carbohydrates, proteins and nucleic acids.

PG3 PHAC10Physical Chemistry- III (Advanced Topics in Physical Chemistry)

Objectives:

- The objective is to study the basics of electrochemistry and its importance to modern industry and technology.
- To give an in-depth account of different theories of reaction rates, kinetics of fast reactions and reaction in solution.
- To study the chemistry of surfaces and various techniques employed for the characterization of different types of surface phenomena and the importance of adsorption process and catalytic activity at the solid surfaces.
- To recognize the general properties of colloids and macromolecules.
- To study the different types of quantum statistics and its comparison, Laws related to heat capacity of solids, phase transition and thermionic emission.
- To acquire knowledge of photochemistry and photophysical principles, their applications

Outcome:

- Understand theories of ions in solutions.
- Apply the theories to explain the variation of ionic conductance with concentration, electric field.
- The student will acquire knowledge about different theories on reaction rate, can analyse the mechanistic path and the experimental conditions of different types of reactions.

- Will able to understand the different techniques for analysing fast reactions.
- Will appreciate the applications of chemical principles of surface catalysis and colloidal chemistry in industrial synthesis.
- Able to classify colloids present in nature apply its properties in daily life.
- Apply the principles of adsorption in daily life situations.
- The student will able to apply photochemistry and photophysical principles on environmental and biological processes and will explain photophysical energy conversion to generate electricity
- Gains numerical ability and analysing power to solve problems.

PG3PHA C11Medicinal Chemistry I (Drug Design and Pharmacologcy)

Aim: This course is designed to impart a fundamental knowledge on the preparatory pharmaceutical chemistry of preparing the different conventional dosage forms. The main purpose of the area pharmacology is to understand what drugs do to the living organisms and how their effects can be applied to therapeutics. The subject covers the information about the drugs like, mechanism of action, physiological and biochemical effects (pharmacodynamics) as well as absorption, distribution, metabolism and excretion (pharmacokinetics) along with the adverse effects, clinical uses, interactions, doses, contraindications and routes of administration of different classes of drugs.

Objectives: Upon completion of this session the student should be able to

- Understand the pharmacological actions of different categories of drugs
- This subject deals with the monographs of inorganic drugs and pharmaceuticals.
- understand the medicinal and pharmaceutical importance of inorganic compounds
- Understand the basics of different dosage forms, pharmaceutical incompatibilities and pharmaceutical calculations.
- Apply the basic pharmacological knowledge in the prevention and treatment of various diseases.
- Understand the professional way of handling the prescription
- Preparation of various conventional dosage forms

PG3 PHA C12 Spectroscopic Methods in Chemistry

Course Objectives:

- To understand the basic ideas of different spectroscopic Techniques
- To identify the compounds by analyzing the UV, IR NMR and Mass spectrum
- To interpret the spectrum of organic compounds
- To develop the structure elucidation skill of organic compounds using different types of spectral data

Outcome:

- Achieve advanced knowledge about the interactions of electromagnetic radiation and matter and their applications in spectroscopy.
- To understand the selection rules of UV-Visible spectroscopy and learn the various rules to calculate the absorption maxima.
- Study the chirooptical properties and do the problems
- be able to analyse and interpret IR spectroscopic data based on stereochemistry and various factors influencing the spectra study the basic principles of NMR and factors influencing spectra and understand the advanced topics like two dimensional spectroscopy.

- Study mass spectroscopic techniques and problems based on it.
- Be able to solve problems related to the structure and to study molecular interactions by choosing suitable spectroscopic methods and interpreting corresponding data.

PG4PHA E01 Bacteriology and Biochemistry

Aim: This subject is designed to impart fundamental knowledge on the various microorganisms and general principles of microbial control, immunity, structure and chemistry of amino acids, proteins and nucleic acids enzymes and hormones. The scope of the subject is providing biochemical facts and the principles to understand metabolism of nutrient molecules in physiological and pathological conditions. The subject emphasizes on biological oxidation and electron transport chains The syllabus also emphasizes on the study of composition of blood cells and regulation of acid base balance.

Objectives: Upon completion of this session student shall be able to

- Understand the various microorganisms, their growth requirements, staining techniques and general principles of microbial control.
- Understand the various types of immunity, antigen - antibodies reactions and various types of vaccines.
- Understand the catalytic role of enzymes, importance of enzyme inhibitors in design of new drugs, therapeutic and diagnostic applications of enzymes.
- Understand the role of hormones.
- Understand the metabolism of nutrient molecules in physiological and pathological conditions.
- Understand the genetic organization of mammalian genome and functions of DNA in the synthesis of RNAs and proteins.
- Understand the biological oxidation and electron transport chains.
- Understand the Blood groups and the composition blood cells.
- Understand the Blood clotting- factors and mechanism.
- Understand the Regulation of acid base balance
- To understand the importance of metabolism of substrates.
- Will acquire chemistry and biological importance of biological macromolecules.
- To acquire knowledge in qualitative and quantitative estimation of the biological macromolecules.
- To know the interpretation of data emanating from a Clinical Test Lab.
- To know how physiological conditions influence the structures and re-activities of biomolecules.
- To understand the basic principles of protein and polysaccharide structure. Students will be able to acquire, articulate, retain and apply specialized language and knowledge relevant to microbiology.

PG4PHA E02 PHARMACOGNOSY & PHARMACEUTICAL OPERATIONS

Aims and Objectives

- In this module, students will learn about the Pharmacognosy of official drugs used in pharmacy. various principles of dispensing medicaments
- Identify drug from natural origin and their supply, cultivation, collection, storage along with their aspecial conditions

PG4 PHA E03 Medicinal Chemistry II

Aim: This subject is designed to impart fundamental knowledge on the structure, chemistry and therapeutic value of drugs. The subject emphasizes on structure activity relationships of drugs, importance of physicochemical properties and metabolism of drugs. The syllabus also emphasizes on chemical synthesis of important drugs under each class.

Objectives: Upon completion of the session the student shall be able to

- understand the chemistry of drugs with respect to their pharmacological activity
- understand the drug metabolic pathways, adverse effect and therapeutic value of drugs
- know the Structural Activity Relationship (SAR) of different class of drugs
- write the chemical synthesis of some drugs

Course Content

Study of the development of the following classes of drugs, Classification, mechanism of action, uses of drugs mentioned in the course, Structure activity relationship of selective class of drugs as specified in the course and synthesis of drugs.

PG4PHA E01 Elective 1 Bacteriology and Biochemistry

Aim: Biochemistry deals with complete understanding of the molecular levels of the chemical process associated with living cells. The scope of the subject is providing biochemical facts and the principles to understand metabolism of nutrient molecules in physiological and pathological conditions.

Objectives: Upon completion of this session student shall be able to

- Understand the catalytic role of enzymes, importance of enzyme inhibitors in design of new drugs, therapeutic and diagnostic applications of enzymes.
- Understand the metabolism of nutrient molecules in physiological and pathological conditions.
- Understand the genetic organization of mammalian genome and functions of DNA in the synthesis of RNAs and proteins.
-

PG4PHA P04 PHARMACEUTICAL ANALYSIS PRACTICAL

Aim: This practical session deals with the fundamentals of analytical chemistry and principles of electrochemical analysis of drugs

Objectives: Upon completion the student shall be able to

- understand the principles of volumetric and electro chemical analysis
- carryout various volumetric and electrochemical titrations
- develop analytical skills

PG4PHA P05 DRUG SYNTHESIS AND DISPENSING PRACTICAL

Course outcomes:

1. To synthesise of drugs and drug intermediate through multi-step organic syntheses.
2. To perform the organic synthesis using green alternatives of the conventional chemical methods.
3. To synthesise organic compound using microwave assisted organic syntheses.
4. To analyse and predict the FTIR, ^{1}H and ^{13}C NMR spectra of the intermediates and products at each stage of synthesis by the above methods.
5. To carry out the dispensing of emulsions, liniments and mixtures involving incompatibilities.

PG4PHAP06 BIOCHEMISTRY AND BACTERIOLOGY PRACTICAL

Aim: This practical session deals with the fundamentals of analytical chemistry for the analysis of blood, urine, milk and water and isolation techniques of phytochemicals from their natural sources. This practical session also deals with the preparation of some typical nutrient media for collection and isolation of Bacteria and different Staining techniques for the study of the morphology of the bacteria. .
Objectives: Upon completion the student shall be able to

- Understand the principles of determination of blood group and Rh factor.
- Understand to enumerate RBC, WBC and DC of blood.
- Understand to estimate qualitatively and quantitatively the different components present in the blood, urine , milk and water
- Understand to isolate different phytochemicals from their natural sources.
- Understand to separate mixtures of serum proteins, amino acids and dyes by different techniques.
- Understand to prepare some typical nutrient media for collection and isolation of bacteria.
- Understand the different staining methods for the study of the morphology of the bacteria.
- Understand the Understand the method of study of antibacterial activity of compounds and complexes.
- Students will acquire and demonstrate competency in laboratory safety and in routine and specialized microbiological laboratory skills applicable to microbiological research or clinical methods, including accurately reporting observations and analysis.

- Students will communicate scientific concepts, experimental results and analytical arguments clearly and concisely, both verbally and in writing.
- Students will demonstrate isolation of and identification of microbes.
- Students can able to design microbiology laboratory considering all the aspects of safety
- Students will acquire knowledge about validating the microbiological equipment and reporting the observations
- To understand the importance of metabolism of substrates.
- Will acquire chemistry and biological importance of biological macromolecules.
- To acquire knowledge in qualitative and quantitative estimation of the biological macromolecules.
- To know the interpretation of data emanating from a Clinical Test Lab.
- To know how physiological conditions influence the structures and reactivity's of biomolecules.
- To understand the basic principles of protein and polysaccharide structure.
- Develop analytical skills